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A Lattice Boltzmann approach to plasma simulation in the context of wakefield acceleration

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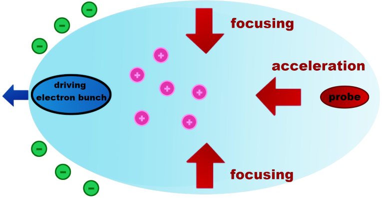
Oct 02, 2024

Plasma Wakefield Acceleration (PWFA)



Relativistic electron bunch injected in a plasma channel

1. Plasma electrons on the bunch trajectory are pushed back
2. A wake of positive charges is formed
3. Strong accelerating/focusing electric fields develop in the wake
4. A probe particle bunch could take advantage of such fields

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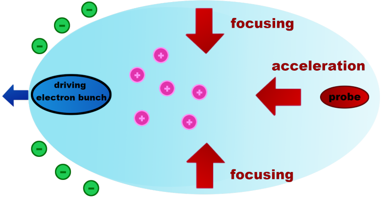

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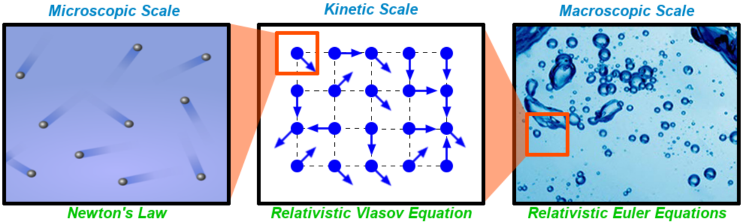
Plasma modeling achieved at different space scales:

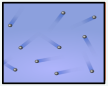


Target equation: **relativistic Vlasov equation**

$$\frac{d}{dt} f(\mathbf{r}, \mathbf{v}, t) = \cancel{\Omega(\mathbf{r}, \mathbf{v}, t)} = 0$$

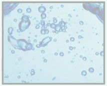
Approaches to theoretical/numerical modeling in PWFA

Kinetic Solvers (PIC)



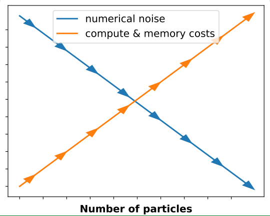
Solutions to kinetic equations via bottom-up simulations of Lagrangian particles

Fluid Models

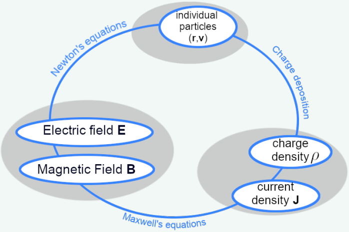


Coarse grained theories that solve for the first moments of the kinetic distribution function

1. **All** kinetic effects are included
2. Averaging over particles brings in **numerical noise**
3. **Computational costs** increase with number of particles



The PIC loop

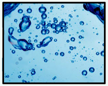


Approaches to theoretical/numerical modeling in PWFA

Kinetic Solvers (PIC)

Solutions to kinetic equations via bottom-up simulations of Lagrangian particles

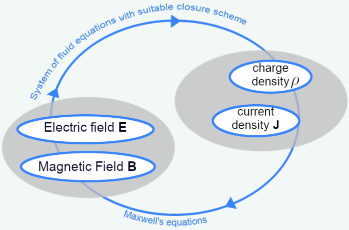
Fluid Models



Coarse grained theories that solve for the first moments of the kinetic distribution function

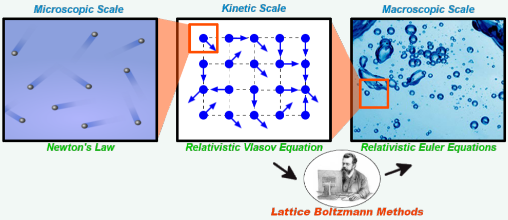
1. Approximated theory: **looses some kinetic effects**
2. By construction, **no numerical noise**
3. Moments equations need to be **properly closed**

The fluid loop



Approaches to theoretical/numerical modeling in PWFA

Lattice Boltzmann Methods (LBM)



What it does:

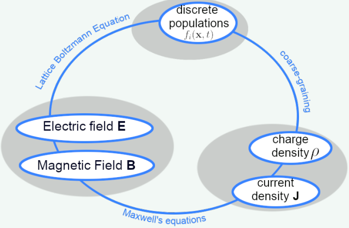
Provides a fluid (and not only!) description of the system via a **suitable discretization** of the kinetic momentum space

$$f(\mathbf{x}, \mathbf{p}, t)$$

Our Goal:

To develop a computational tool for enabling **realistic** and **rapid** fluid simulations of PWFA processes amenable to **kinetic extensions**

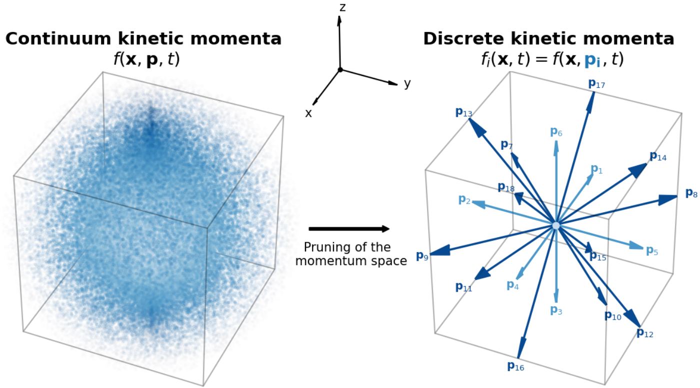
The LBM loop



Further details in **Parise et al.** *Physics of Plasma* (2022) & **Simeoni et al.** *Physics of Plasma* (2024)

Key aspects of the method [1,2]: momentum-space discretization

Suitable discretization of the momentum space via adoption of **quadrature rules**...



How do we select such discrete momenta?

[1] Succi *The Lattice Boltzmann Equation: For Complex States of Flowing Matter*, Oxford University Press, (2018)

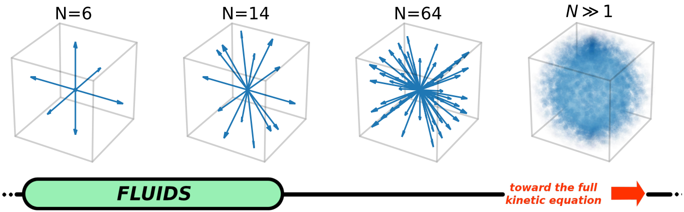
[2] Krüger et al. *The Lattice Boltzmann Method*, Springer International Publishing, (2017)

Key aspects of the method [1,2]: momentum-space discretization

Choice made to preserve **exactly** the continuous moments of the p.d.f when moving to a discrete momentum space

$$\rho, \mathbf{J} = \underbrace{\int \left[(\dots) f(\mathbf{x}, \mathbf{p}, t) \right] d\mathbf{p}}_{\text{CONTINUUM MOMENTUM SPACE}} = \underbrace{\sum_{i=0}^{N-1} \left[(\dots) f_i(\mathbf{x}, \mathbf{p}_i, t) \right]}_{\text{DISCRETE MOMENTUM SPACE}}$$

How many discrete momenta N to take?
It depends on the number of moments one wants to recover!
$N \sim O(10)$ for fluid modeling



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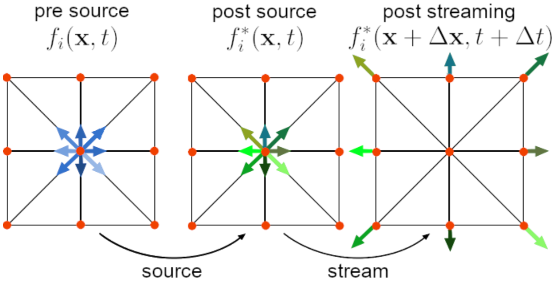
Key aspects of the method [1,2]: space - time discretization

- Obtain the **LB Equation**

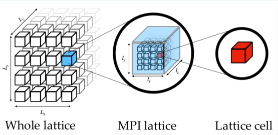
$$f_i\left(\mathbf{x}+\Delta\mathbf{x}, t+\Delta t\right) = f_i(\mathbf{x}, t) + \Delta t \Sigma_i(\mathbf{x}, t)$$

1. Time discretization Δt
2. Regular lattice of characteristic length $\Delta\mathbf{x} = \left(\frac{\mathbf{p}_i}{m}\right)\Delta t$
3. Source term $\Sigma_i(\mathbf{x}, t)$ (Electromagnetic, ...)

- Evolve through **source & stream** paradigm



source & stream paradigm amenable to **multi-core computation**



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The fluid closure problem

$$\frac{d}{dt} f(\mathbf{r}, \mathbf{v}, t) = 0 \quad \Longrightarrow$$

- Conservation of mass
- Conservation of momentum
- Conservation of energy

Set of equations not yet closed. **Fluid closure is needed**

COLD CLOSURE

Zero temperature limit ($T = 0$)

$\Downarrow$

$$\boldsymbol{\sigma} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

LOCAL EQ. CLOSURE [1] (LEC)

Relativistic Maxwellian equilibrium ($f = f^{eq}$)

$\Downarrow$

Entropy conservation

$\Downarrow$

$$\boldsymbol{\sigma} = \begin{pmatrix} P & 0 & 0 \\ 0 & P & 0 \\ 0 & 0 & P \end{pmatrix}$$

WARM CLOSURE [2,3](WARMC)

Truncation of III order centralized moment

$\Downarrow$

$$\boldsymbol{\sigma} = \begin{pmatrix} P_\perp & 0 & 0 \\ 0 & P_\perp & 0 \\ 0 & 0 & P_\parallel \end{pmatrix}$$

[1] Toepfer et al. *Phys. Rev. A* (1971)
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Truncation of III order
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Our Lattice Boltzmann code is equipped to work with **all** of theese closures

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WARM CLOSURE (WARMC)

$$\boldsymbol{\sigma} = \begin{pmatrix} P_\perp & 0 & 0 \\ 0 & P_\perp & 0 \\ 0 & 0 & P_\parallel \end{pmatrix}$$

Relevant features in the context of warm PWFA...

- **Wave breaking** (regularization of singularity of the cold fluids) [1,2,4]
- Impact on late stage dynamics: **acoustic waves & motion of ions** [5]
- **Cumulative heating** from the acceleration of long bunch trains [5]
- **Broadening** of electron filaments in positron acceleration experiments [6]

[1] Schroeder et al. *Phys. Rev. E*, (2005)-(2010)

[2] Katsouleas et al. *Phys. Rev. Lett.* (1988)

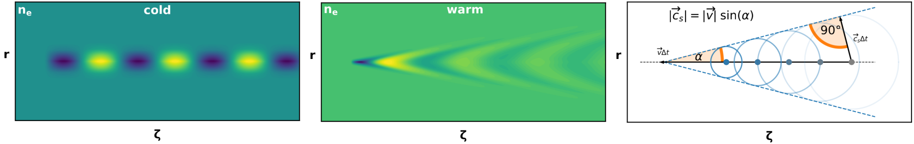
[3] Toepfer *Phys. Rev. A* (1971)

[4] Rosenzweig *Phys. Rev. A Gen. Phys.* (1988)

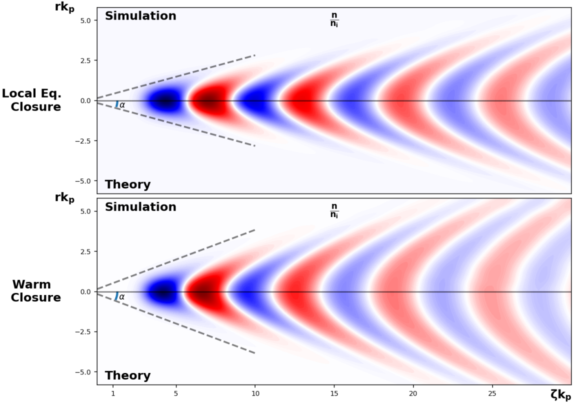
[5] D'Arcy et al. *Nature* (2022)

[6] Diederichs et al. *Physics of Plasmas* (2023)

Results in warm linear theory: acoustic waves



When the driver's perturbation is weak, we have a linear theory to confront with...



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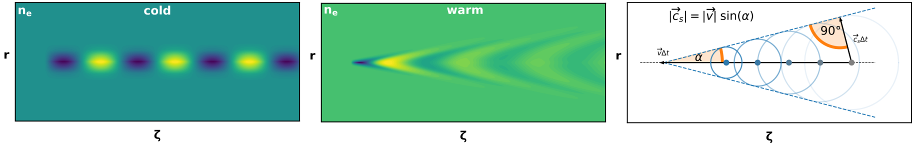
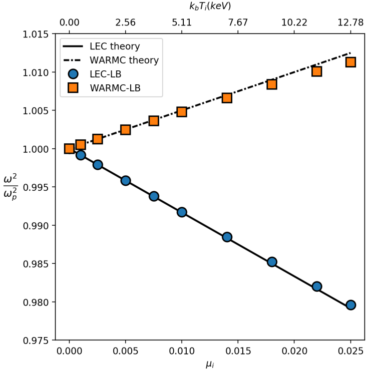
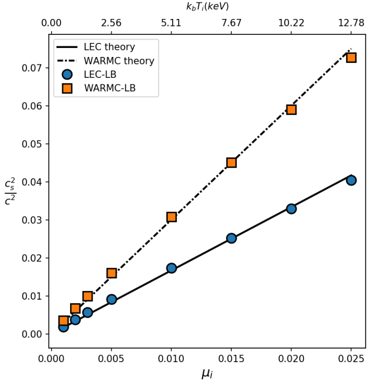


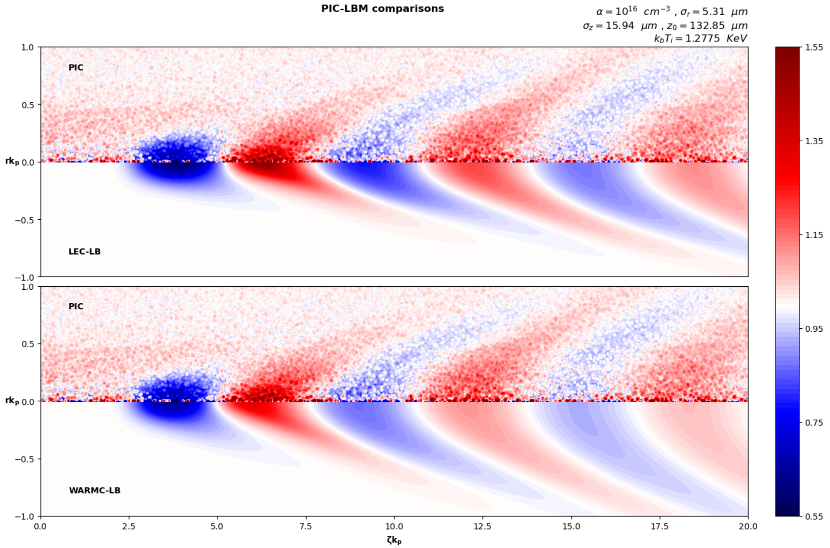
...and can measure temperature/closure dependent parameters





Results: PIC comparisons

Can we use PIC solvers to discern between the two fluid closures?



NO: too noisy to perform precision measures

Results: pressure anisotropies

COLD CLOSURE

$$\boldsymbol{\sigma} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

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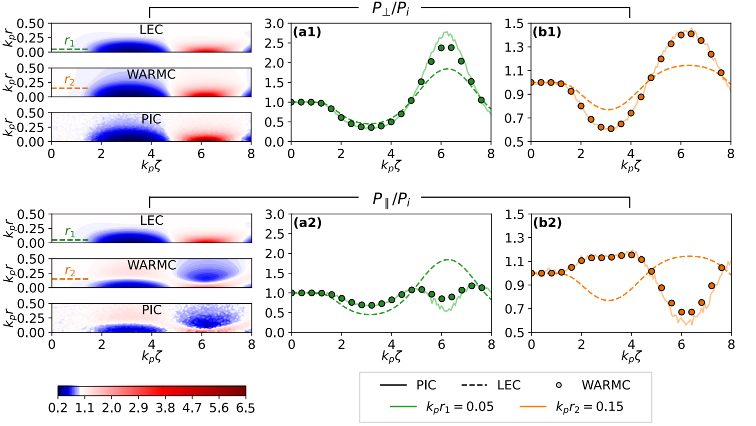


Further details in **Simeoni et al.** *Physics of Plasma* (2024)

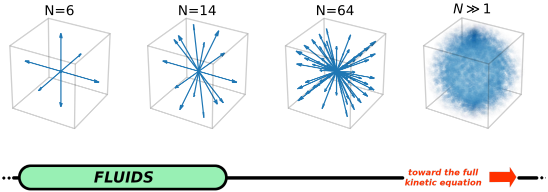
Outlook & Conclusions

First step forward in the development of a a computational tool for enabling **realistic** and **rapid** prototyping for PWFA.

- Plasma treatment based on the lattice Boltzmann method
- Capability to include thermal effects (different fluid closures)

What's next?

1. In depth comparison with PICs for quantitative assessments
2. GPU porting and Open Access
3. Extend methodology to full kinetic eqs.



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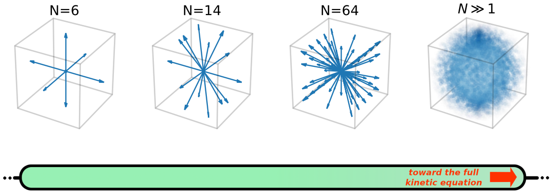


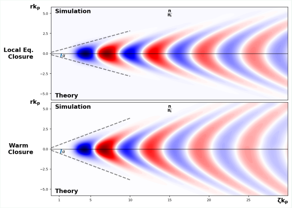
Thank You!

- Parise et al., **Lattice Boltzmann simulations of plasma wakefield acceleration**, *Physics of Plasmas*, (2022) 10.1063/5.0085192
- Simeoni et al., **Lattice Boltzmann method for warm fluid simulations of plasma wakefield acceleration**, *Physics of Plasmas*, (2024) 10.1063/5.0175910
- Simeoni et al., **Thermal fluid closures and pressure anisotropies in numerical simulations of plasma wakefield acceleration**, *Physics of Plasmas*, (2024) 10.1063/5.0216707

Backup Slides

Some words on performances...

Representative simulation

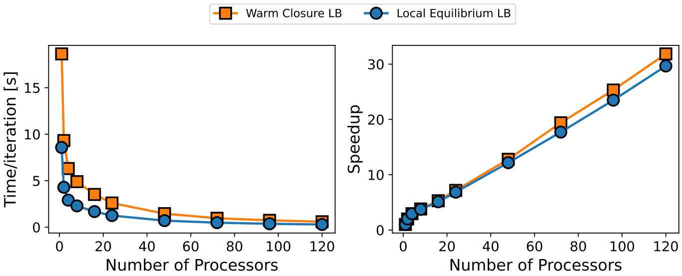


Sim. parameters and running time

- ζ lattice points $= 3 \cdot 10^3$ ($\Delta\zeta = 0.53\ \mu m$)
- r lattice points $= 6 \cdot 10^2$ ($\Delta r = 0.53\ \mu m$)
- total time steps $= 3 \cdot 10^4$ ($\Delta t = 0.17$ fs)
- CPUs = 96 (Intel Xeon E5-2695@2.4 GHz)

$\sim$ 3 hours (Local Equilibrium LB)
$\sim$ 6 hours (Warm Closure LB)

Parallelization on multi CPUs using MPI paradigm



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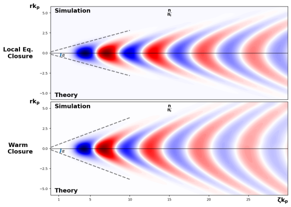

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What about multi GPUs?

Our code is not running (yet!) on GPUs, but there are already LB-GPUs implementations in our research group [1]

Performance for a bi-component system 512^3 with same color gradient model measured in GLUPS running on multiple NVIDIA Ampere A100 GPUs (each card equipped with 80 GB of RAM) and a cluster of nodes made of 2x 20-core 2.4 GHz Intel Xeon Gold 6148 (Skylake) processors. Note the first line is reporting the number of A100 GPU cards and the number of CPU cores for LBcuda and LBSoft, respectively.

	512^3 Grid	1	8	16	32	64 ⟵ number of CPUs/GPUs
LB on GPUs ⟶	LBcuda	1.04	7.63	14.13	23.13	36.05
LB on CPUs ⟶	LBSoft	$1.8 \cdot 10^{-3}$	$13 \cdot 10^{-3}$	$24 \cdot 10^{-3}$	$44 \cdot 10^{-3}$	$86 \cdot 10^{-3}$

[1] Bonaccorso et al. *Computer Physics Communications*, 277:108380, (2022)