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

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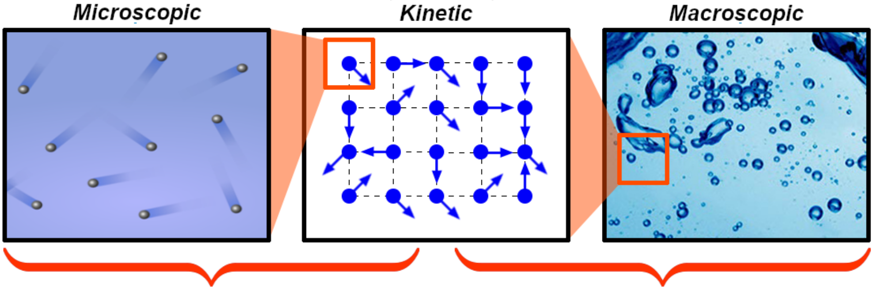
Approaches to PWFA Simulation

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



PIC SOLVERS [1,2,3,4,5]

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

$$\mathbf{F} = \frac{d\mathbf{p}}{dt}$$

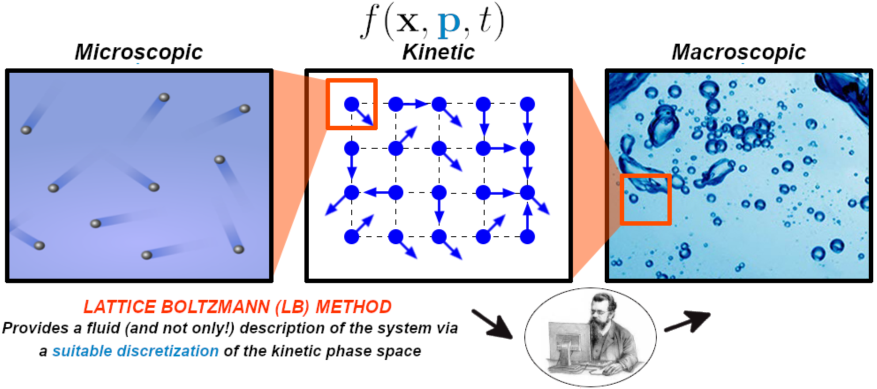
FLUID SOLVERS [6,7,8,9]

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

$$M^{(n)}(\mathbf{x}, t) \propto \int f(\mathbf{x}, \mathbf{p}, t)\mathbf{p}^n d\mathbf{p}$$

[1] Fonseca et al. *Comp. Science ICCS* (2002)
[2] Lehe et al. *Computer Phys. Comm.* (2016)
[3] Burau et al. *IEEE Trans. on Plasma Sc.* (2010)
[4] Benedetti et al. *IEEE Trans. on Plasma Sc.* (2008)
[5] Diederichs et al. *Computer Phys. Comm.* (2022)
[6] Lotov et al. *Phys. Plasmas* (1998)
[7] Benedetti et al. *AIP Conf. Proc.* (2010)
[8] Marocchino et al. *Nucl. Inst. & Meth. in Phys* (2016)
[9] Tomassini et al. *Plasma Phys. and Controlled Fusion* (2015)

Approaches to PWFA Simulation



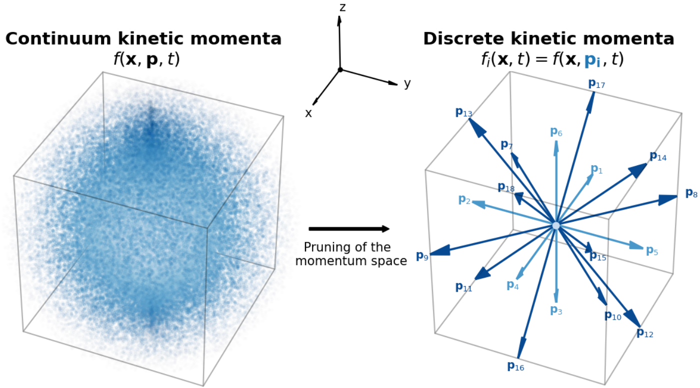
Our Goal

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

Further details in **Simeoni et al.** *arXiv*, 2309.04872, (2023)
& **Gianmarco Parise**'s Poster (poster session Wed 19:00, ID:172)

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)

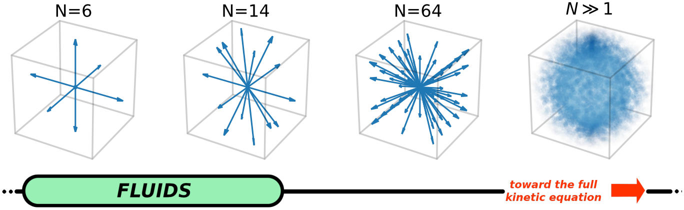
[2] Krüger et al. *The Lattice Boltzmann Method*, Springer International Publishing, (2017)

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

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

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



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

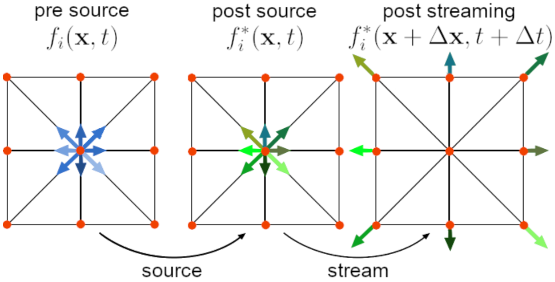
[2] Krüger et al. *The Lattice Boltzmann Method*, Springer International Publishing, (2017)

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

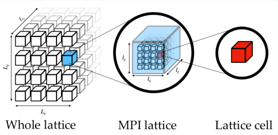
- Obtain the **LB Equation**

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

  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**



How to adapt this framework for fluid modeling?

[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)

Development of a fluid model from kinetic theory [1]

- Start from the **relativistic kinetic equation**

$$p^\alpha \frac{\partial f}{\partial x^\alpha}(\mathbf{x}, t) = \Sigma(\mathbf{x}, t)$$

- Space - time Advection of f
- Source term: electromagnetic interaction ($F^{\alpha\beta}$)

- From here, build the **hydro variables** as the first moments of f...

Particle flow $$N^\alpha = \int f p^\alpha \frac{d\mathbf{p}}{p_0}$$

Energy-momentum tensor $$T^{\alpha\beta} = \int f p^\alpha p^\beta \frac{d\mathbf{p}}{p_0}$$

Energy-momentum flux $$K^{\alpha\beta\gamma} = \int f p^\alpha p^\beta p^\gamma \frac{d\mathbf{p}}{p_0}$$

- ...and express their respective **equations of transfer**:

Mass conservation $$\partial_\alpha N^\alpha = 0$$

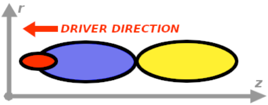
Energy-momentum conservation $$\partial_\alpha T^{\alpha\beta} = \frac{q}{c} F^{\beta\alpha} N_\alpha$$

Energy-momentum flux conservation $$\partial_\alpha K^{\alpha\beta\gamma} = \frac{q}{c}(F^{\beta\alpha} T_\alpha{}^\gamma + F^{\gamma\alpha} T_\alpha{}^\beta)$$

[1] Schroeder et al. *Phys. Rev. E*, 72:055401, (2005) - *Phys. Rev. E*, 81:056403, (2010)

Development of a fluid model from kinetic theory [1]

Set of equations not yet closed. Fluid closure needed!
Quantity of interest:



$$\theta^{\mu\nu} = \int (p^\mu - u^\mu)(p^\nu - u^\nu) f \frac{d\mathbf{p}}{p_0}$$

SECOND ORDER CENTRALIZED MOMENT

COLD CLOSURE	WARM CLOSURE [1,2]	LOCAL EQ. CLOSURE [3]
No thermal spread	Anisotropic thermal spread	Isotropic thermal spread
$\theta^{\mu\nu} = 0$	$\theta^{zz} \neq \theta^{rr}$	$\theta^{zz} = \theta^{rr}$

Many relevant features within context of non-cold closure theories...

- **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 et al. *Phys. Rev. A* (1971)
[4] Rosenzweig *Phys. Rev. A Gen. Phys.* (1998)
[5] D'Arcy et al. *Nature* (2023)
[6] Diederichs et al. *Phys. of Plasmas* (2023)

Enslaving LB to fluid modeling...

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No thermal spread	Anisotropic thermal spread	Isotropic thermal spread
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LB can be adapted for all these closure schemes.
Once proper closure is chosen, fluid eqs. can be recast as Forced Advection eqs...

$$\partial_t A + \nabla \cdot (\mathbf{u}A) = F_A$$

- $A = (N^\alpha, T^{\alpha\beta})$ p.d.f moments
- F_A electromagnetic forcing
- $\mathbf{u}$ fluid transport velocity

LB recovers solution to this eq. by discrete coarse graining [1,2]

$$A = \sum_{i=0}^{N-1} f_i(\mathbf{x}, t)$$

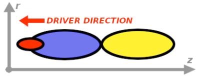
[1] Succi *The Lattice Boltzmann Equation: For Complex States of Flowing Matter*, Oxford University Press, (2018)

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

One example result

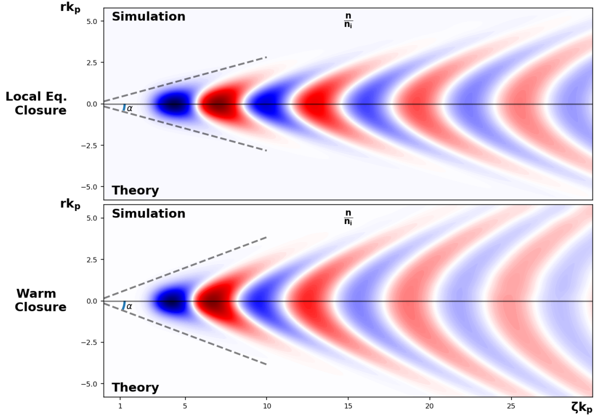
Quantitative assessment of **fluid closures** in PWFA via **spatially resolved warm** plasma simulations

1. Gaussian particle driver
2. Immobile ions
3. 3D axially symmetric-comoving domain



Future Perspective 1

Ion dynamics
↓
acoustic waves
↓
late stage dynamics



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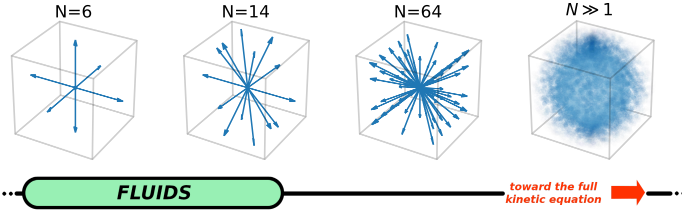
Recovering full Vlasov with LB

Being rooted in kinetic theory, LB can **progressively** be extended to reproduce more and more **kinetic effects**



Already done in contexts other than PWFA (Quark Gluon Plasma [1,2])

Future Perspective 2

Model improvement via **progressive inclusion** of kinetic effects. **Comparisons with PIC** for quantitative assessments.

[1] Ambrus et al. *Phys. Rev. C*, 98:03520, (2018)

[2] Simeoni et al. *Nature Comp. Science*, 2:641, (2022)

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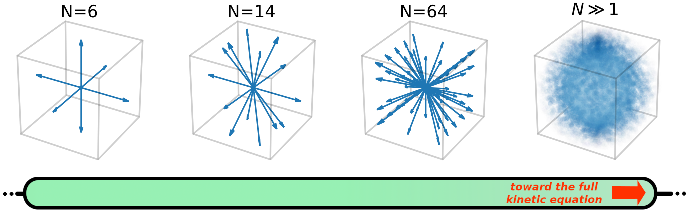

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[2] Simeoni et al. *Nature Comp. Science*, 2:641, (2022)

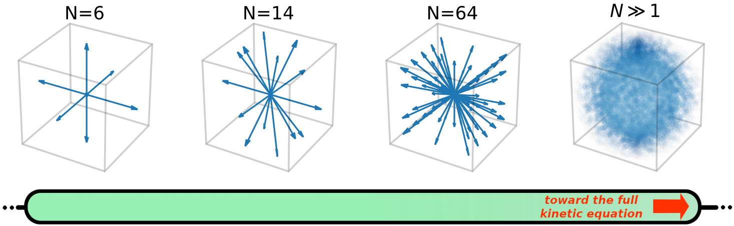
Outlook & Conclusions

First step forward in the development of a a computational tool for enabling **realistic** and **rapid** fluid simulations of PWFA amenable to **kinetic extensions**

- Fluid treatment based on LB
- Capability to include thermal effects (different closures)

What's next?

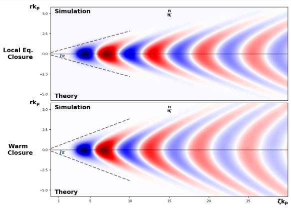
1. Inclusion of ion dynamics
2. Extend methodology to full kinetic eqs.
3. Comparison with PICs for quantitative assessments



Backup Slides

Some words on performances...

Representative simulation

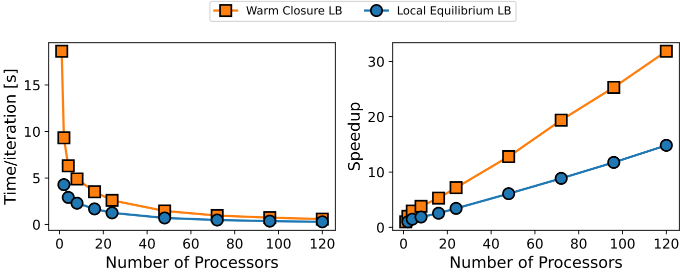


Sim. parameters and running time

- 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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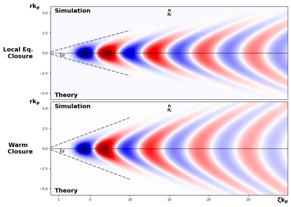

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What about multi GPUs?

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
LBcuda	1.04	7.63	14.13	23.13	36.05
LBSoft	$1.8 \cdot 10^{-3}$	$13 \cdot 10^{-3}$	$24 \cdot 10^{-3}$	$44 \cdot 10^{-3}$	$86 \cdot 10^{-3}$

LB on GPUs → LBcuda
LB on CPUs → LBSoft
← number of CPUs/GPUs

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