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Loading Relativistic Maxwell Distributions in Particle Simulations

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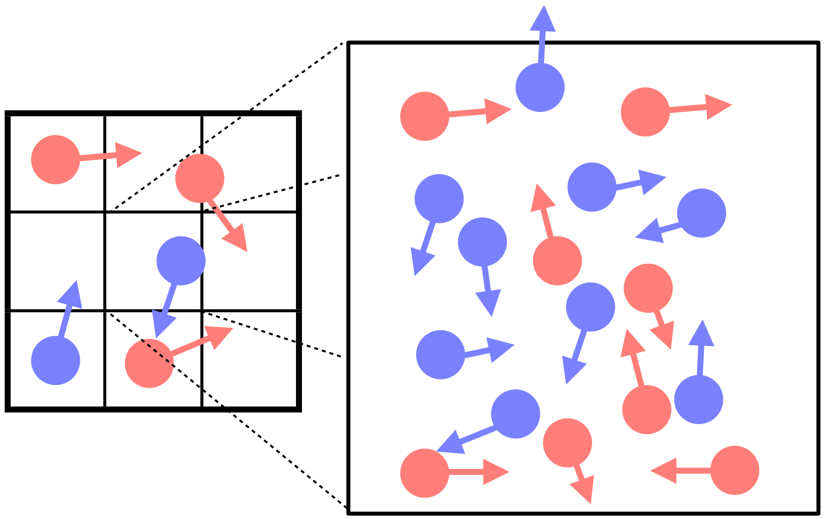
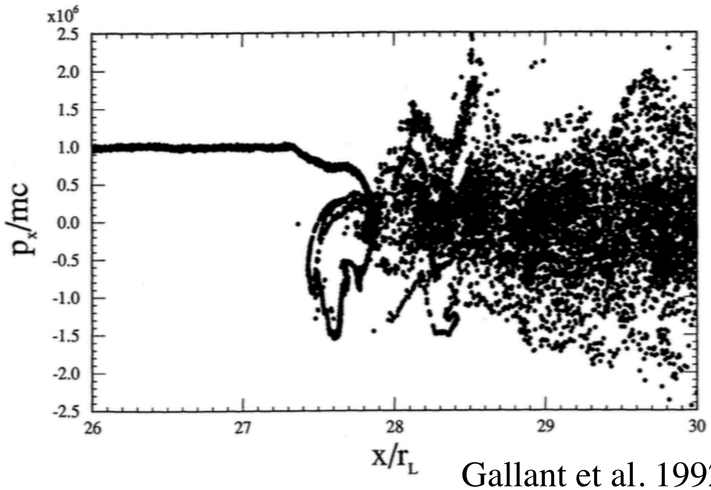
Acknowledgement: T.-N. Kato (NAOJ)

Zenitani, *Phys. Plasmas* **22**, 042116 (2015)

Kinetic modeling of relativistic plasma processes

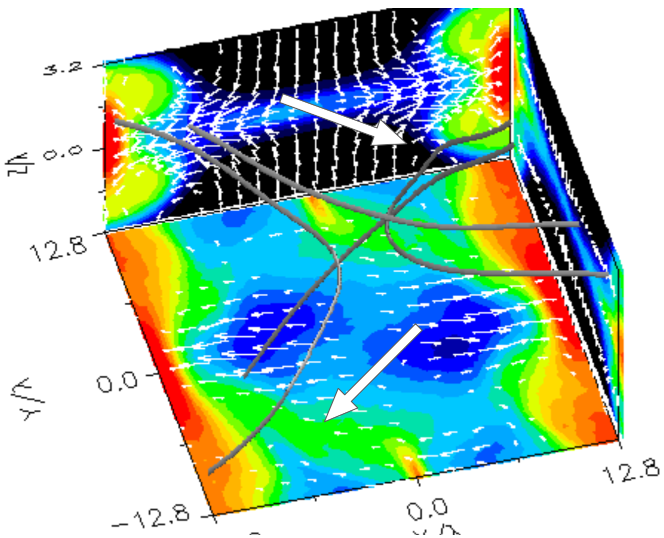


Relativistic shock (90's)



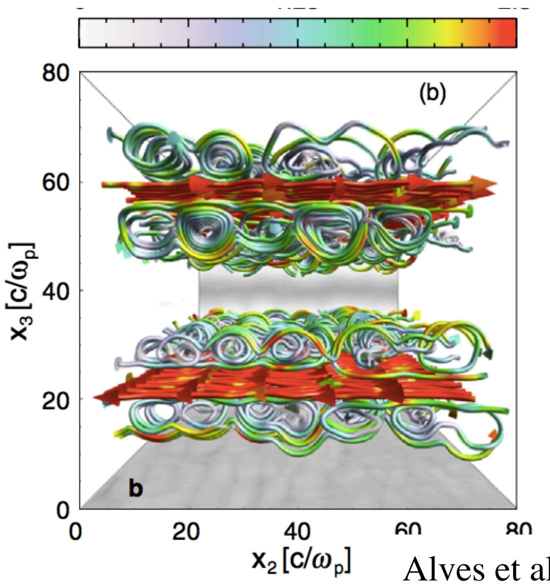
Gallant et al. 1992 *Astrophys. J.*

Relativistic reconnection (00's)



Zenitani & Hoshino 2005 *Phys. Rev. Lett.*

Relativistic flow shear (10's)



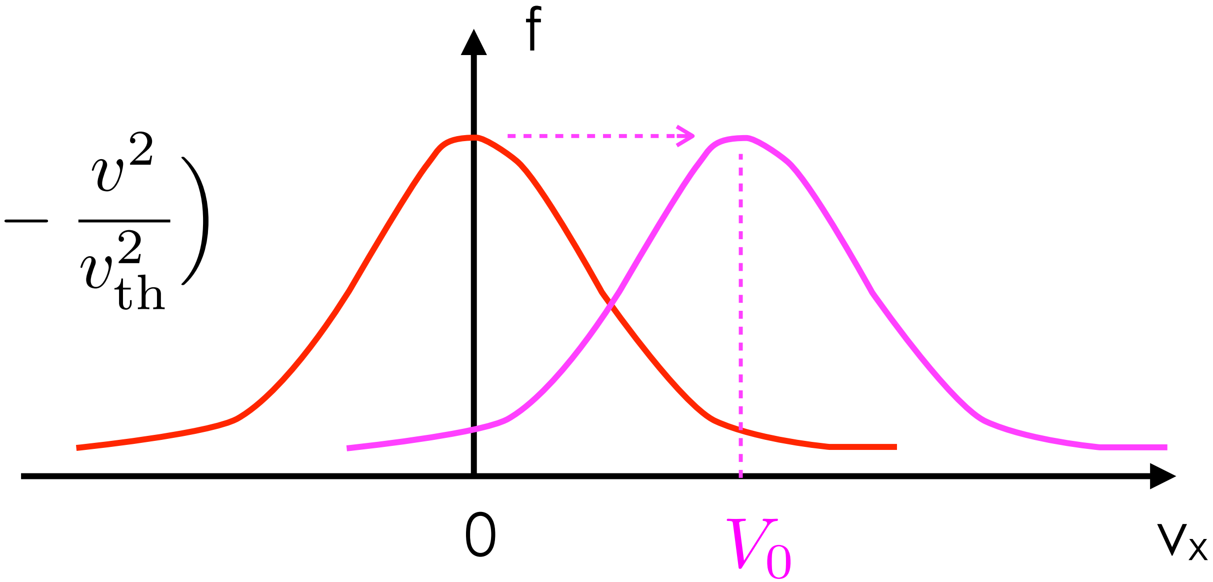
Alves et al. 2012 *Astrophys. J.*

Three technical barriers in relativistic PIC simulations

- 1. Setup
  - Loading velocity distribution functions by using random variables
  - Usually undocumented
- 2. Computation
  - Electromagnetic field (Haber 1974, Vay+ 2011)
  - Particle (Vay 2008)
- 3. Diagnosis & Interpretation
  - Presented in ASJ 2015a meeting (SZ 2015d in prep.)

Nonrelativistic Maxwell distributions

$$f(\boldsymbol{v}) \propto \exp\left(-\frac{v^2}{v_{\rm th}^2}\right)$$



- Uniform variable

$$X_n \ (0 < X_n < 1)$$

- Box=Muller (1958) transform

$$v_x = \sqrt{-2\ln X_1}\sin(2\pi X_2)$$

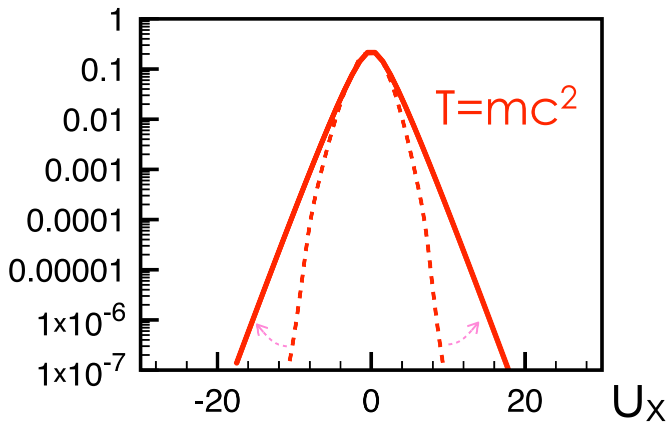
$$v_y = \sqrt{-2\ln X_1}\cos(2\pi X_2)$$

- Galilei transform

$$v_x \leftarrow v_x + V_0$$

Relativistic Maxwell distributions

- Jüttner=Synge distribution

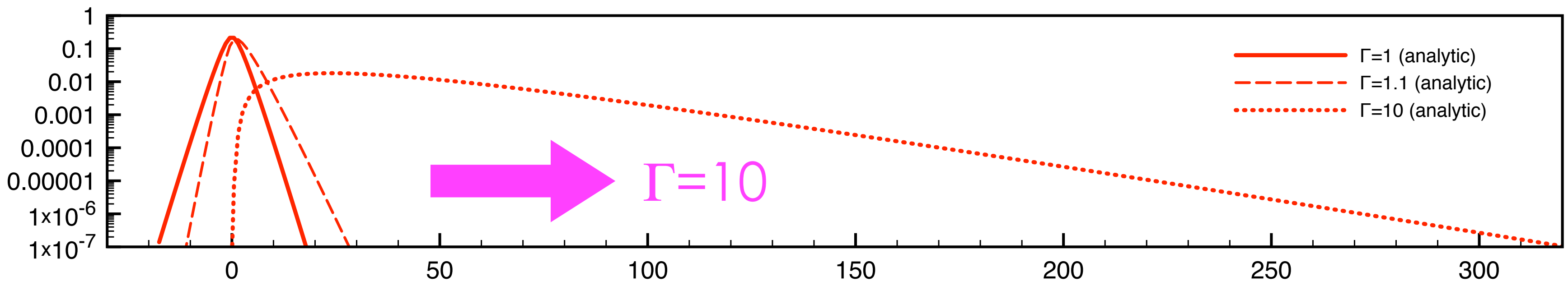


$$f(\boldsymbol{u})d^3u \propto \exp\left(-\frac{\gamma mc^2}{T}\right)d^3u$$
$$\propto \exp\left(-\frac{mc^2\sqrt{1+(u/c)^2}}{T}\right)d^3u$$

$$\boldsymbol{u} = \gamma \boldsymbol{v} \qquad \gamma = [1-(\boldsymbol{v}/c)^2]^{-1/2}$$

- Shifted Maxwell distribution

$$\propto \exp\left(-\frac{\Gamma(\gamma' - \beta u'_x)}{T}\right)d^3u'$$



Recent attempts

- Swisdak (2013) -- Two-step rejection method (Shown on p.15)
- Melzani+ (2013) -- Cylindrical transformation + numerical table

Our strategy

- Stationary Maxwellian
  - Inverse transform method
  - Sobol (1976) method
- Lorentz boost → relativistic shifted Maxwellian
  - Rejection method - 50% efficiency for the stationary case
  - Flipping method - 100% efficiency

Sobol method

[Sobol 1976, Pozdnyakov+ 1977, 1983]

- Spherical form

$$f(u)du \propto \exp\left(-\frac{\sqrt{1+u^2}}{T}\right)u^2du$$

m=1, c=1...

- Gamma (Earlang) distribution

$$P(u;3,T) \propto \exp\left(-\frac{u}{T}\right)u^2 \qquad u = -T\ln X_1X_2X_3$$

- Rejection method

$$\exp\left(\frac{u-\sqrt{1+u^2}}{T}\right) > X_4$$

- Spherical scattering

$$u_x = u\ (2X_5 - 1)$$

$$u_y = 2u\sqrt{X_5(1-X_5)}\cos(2\pi X_6)$$

$$u_z = 2u\sqrt{X_5(1-X_5)}\sin(2\pi X_6)$$

- Another form

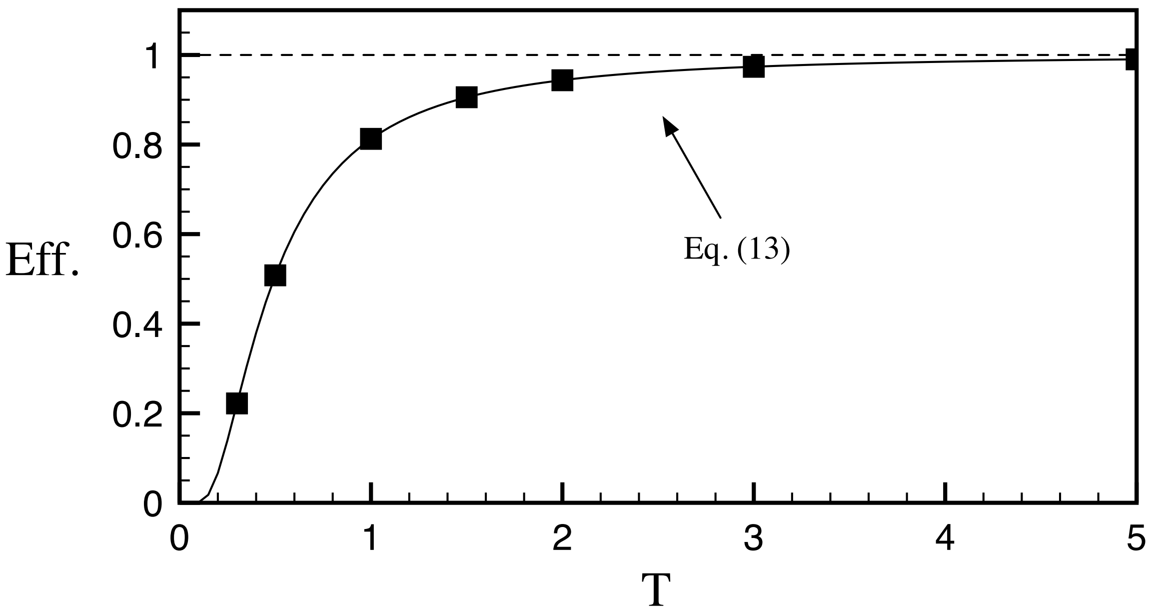
[Pozdnyakov+ 1977]

$$\eta^2 - u^2 > 1$$

$$\eta = -T\ln X_1X_2X_3X_4$$

Loading efficiency

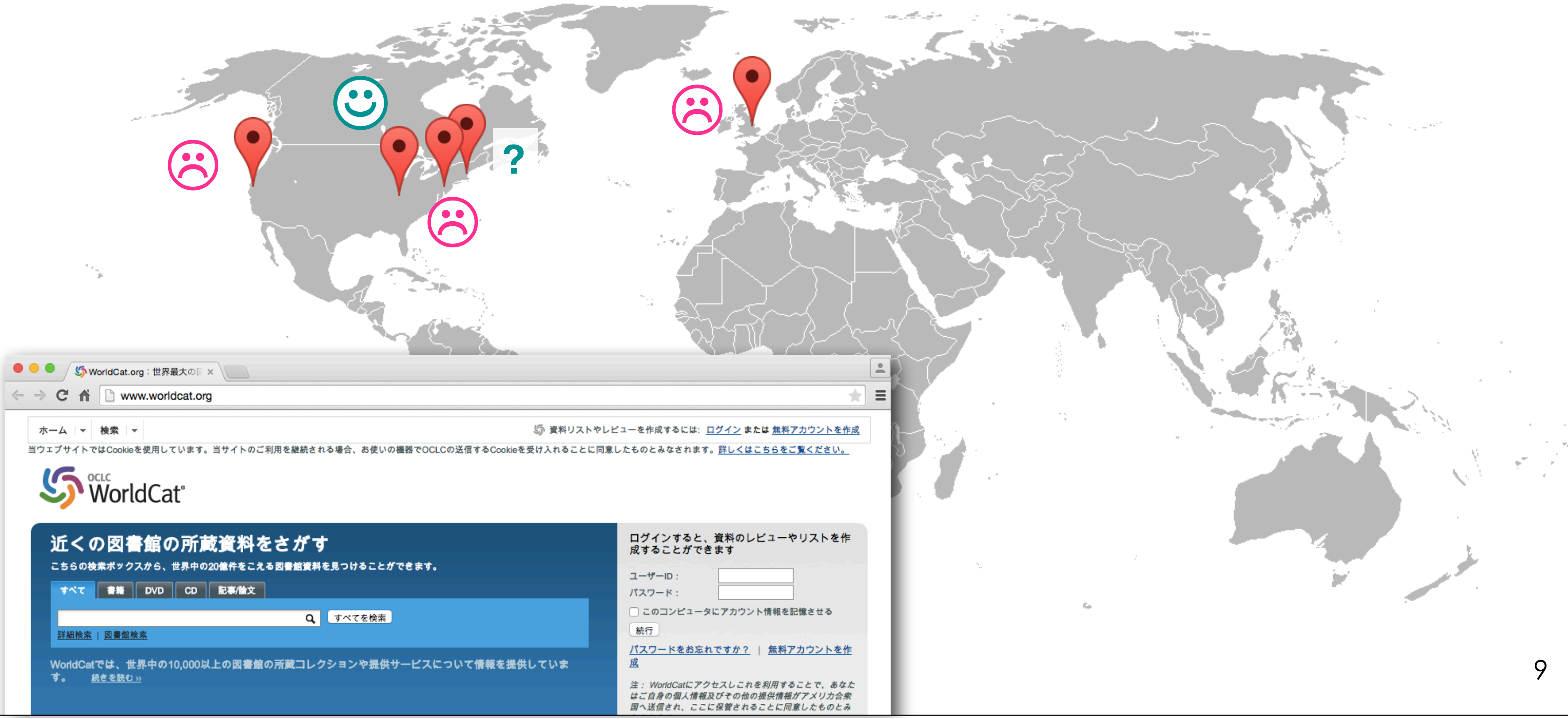
- Efficiency quickly decreases for T << 1
  - We should revert to alternative methods (SZ 2015)



$$\frac{1}{2T^2} K_2(1/T)$$

Quest for the original article

- OCLC/WorldCat database suggested 5 libraries
- We found it at U. Illinois Urbana-Champaign at the 4th attempt



Sobol (1976)'s article

?

И.М.Соболь

О МОДЕЛИРОВАНИИ НЕКОТОРЫХ РАСПРЕДЕЛЕНИЙ,
СХОДНЫХ С ГАММА-РАСПРЕДЕЛЕНИЕМ

Рассмотрим два нестандартных приема для моделирования случайных величин с плотностями вида

$$p(x) = B_n \, x^n \, e^{-b\sqrt{1+x^2}} \qquad (1)$$

и

$$p(x) = C_n \, x^n (e^{bx} - 1)^{-1}, \qquad (2)$$

где $0 < x < \infty, b > 0$, а B_n и C_n – нормировочные постоянные. Эти приемы позволяют, в частности, моделировать импульсы релятивистских электронов и частоты фотонов; они использовались в работе [I].

- He did it right 40 years ago...

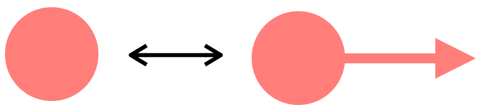
52. "Infinite-Dimensional Uniformly Distributed Sequences in Monte Carlo Algorithms," in *Monte Carlo Methods in Computational Mathematics and Mathematical Physics* (Novosibirsk, 1974), pp. 24–31 [in Russian].

59. "On Simulation of Certain Distributions Similar to Gamma Distribution," in *Monte Carlo Methods in Computational Mathematics and Mathematical Physics* (Novosibirsk, 1976), pp. 24–29 [in Russian].

Lorentz transformation

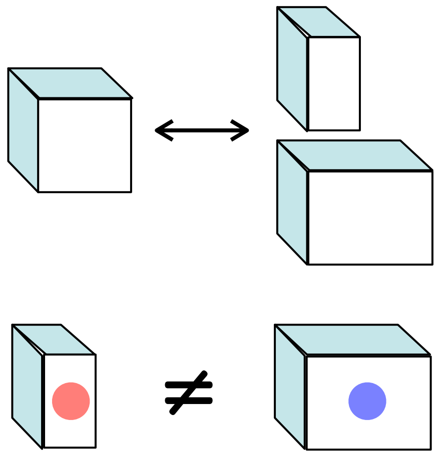
- Energy-momentum
  - Straightforward

$$\begin{aligned} \gamma' &\leftarrow \Gamma(\gamma + \beta u_x) \\ u_x' &\leftarrow \Gamma(u_x + \beta\gamma) \\ u_y' &\leftarrow u_y \\ u_z' &\leftarrow u_z \end{aligned}$$



- Space-time
  - Contraction of a volume element

$$f'(\boldsymbol{u}')d^3u' = f(\boldsymbol{u})\left(\frac{\gamma'}{\gamma}\right)d^3u$$

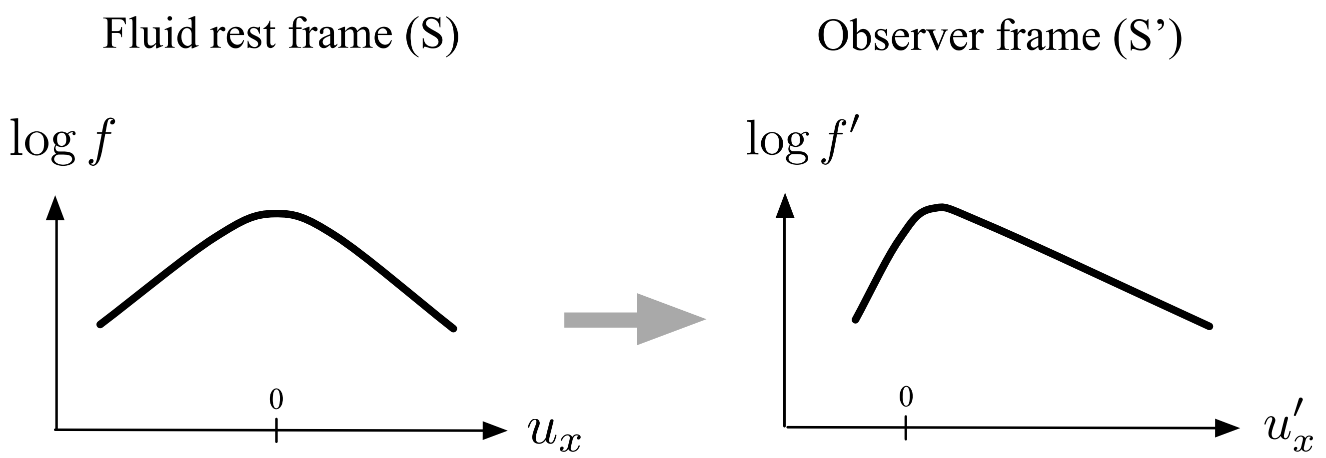


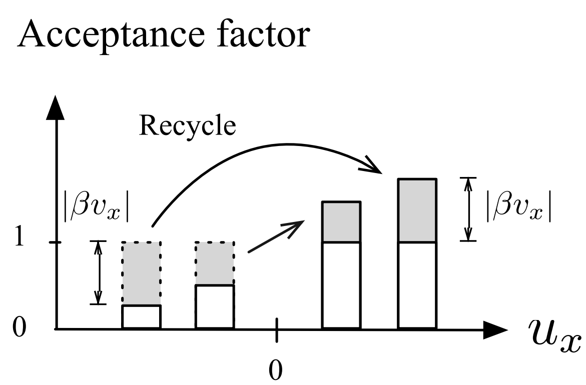
Volume transform factor

$$\frac{\gamma'}{\gamma} = \Gamma(1 + \beta v_x)$$

- Undocumented workarounds
  - 1. Do nothing (incorrect result)
  - 2. Analytic formula (CfCA, Colorado)
  - 3. Adjust particle density (SZ, 4D2U)
  - 4. Adjust particle weight (Harvard)

Volume transform - Flipping method



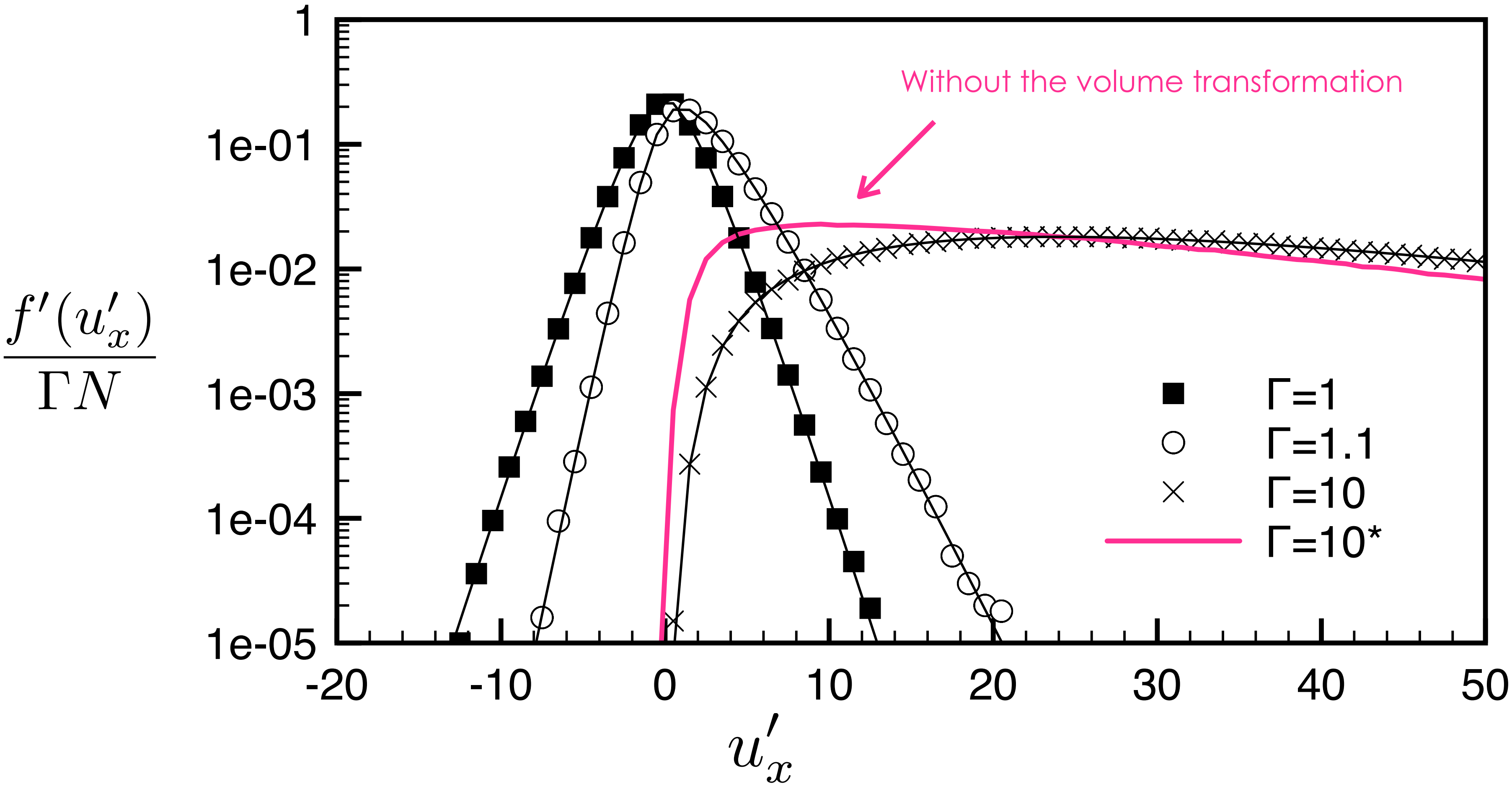


Volume transform factor
(rescaled by $1/\Gamma$)

$$\frac{1}{\Gamma}\left(\frac{\gamma'}{\gamma}\right) = (1 + \beta v_x)$$

- One can adjust the density by recycling the grey part in arbitrary $V_x(U_x)$-symmetric distributions

Numerical test



- Excellent agreement between numerical results vs analytic curve
- Volume transform factor corrects energy flux by ~25%

Summary

- Stationary Maxwellian
  - Inverse transform method
  - Sobol (1976) method
- Lorentz boost
  - Rejection method
  - Flipping method
- Let's get started in relativistic PIC simulations

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repeat

  generate X_1, X_2, X_3, X_4, uniform on $(0,\ 1]$

  $u \leftarrow -T \ln X_1 X_2 X_3$

  $\eta \leftarrow -T \ln X_1 X_2 X_3 X_4$

until $\eta^2 - u^2 > 1.$

generate X_5, X_6, X_7, uniform on $[0,\ 1]$

$u_x \leftarrow u\ (2X_5 - 1)$

$u_y \leftarrow 2u\sqrt{X_5(1-X_5)}\cos(2\pi X_6)$

$u_z \leftarrow 2u\sqrt{X_5(1-X_5)}\sin(2\pi X_6)$

if $(-\beta v_x > X_7)$, $u_x \leftarrow -u_x$

$u_x \leftarrow \Gamma(u_x + \beta\sqrt{1+u^2})$

return u_x, u_y, u_z

- More detail:
  - Zenitani, *Phys. Plasmas* **22**, 042116 (2015)

Pseudo codes

Sobol=Zenitani (2015)

repeat
  generate X_1, X_2, X_3, X_4, uniform on $(0, 1]$
  $u \leftarrow -T \ln X_1 X_2 X_3$
  $\eta \leftarrow -T \ln X_1 X_2 X_3 X_4$
until $\eta^2 - u^2 > 1$.
generate X_5, X_6, X_7, uniform on $[0, 1]$
$u_x \leftarrow u\ (2X_5 - 1)$
$u_y \leftarrow 2u\sqrt{X_5(1-X_5)}\cos(2\pi X_6)$
$u_z \leftarrow 2u\sqrt{X_5(1-X_5)}\sin(2\pi X_6)$
if $(-\beta v_x > X_7)$, $u_x \leftarrow -u_x$
$u_x \leftarrow \Gamma(u_x + \beta\sqrt{1+u^2})$
return u_x, u_y, u_z

Zenitani 2015

Nonrelativistic: Box=Muller (1958)

generate X_1, X_2, X_3, X_4, uniform on $[0, 1]$
$v_x \leftarrow \sqrt{-2\ln X_1}\sin(2\pi X_2)$
$v_y \leftarrow \sqrt{-2\ln X_1}\cos(2\pi X_2)$
$v_z \leftarrow \sqrt{-2\ln X_3}\sin(2\pi X_4)$
$v_x \leftarrow (v_x + V_0)$
return v_x, v_y, v_z

Swisdak's two-step method (2013)

Require: p_m is the mode of f
p_+ and p_- satisfy $f(p_\pm) = f(p_m)/e$
$\lambda_+ \leftarrow -f(p_+)/f'(p_+)$, $\lambda_- \leftarrow f(p_-)/f'(p_-)$ {can be re-written in terms of $(\log f)'$}
$q_- \leftarrow \frac{\lambda_-}{p_+ - p_-}$, $q_+ \leftarrow \frac{\lambda_+}{p_+ - p_-}$, $q_m \leftarrow 1 - (q_+ + q_-)$
repeat
generate U and V, uniform variates on $[0, 1]$
if $U \le q_m$ **then**
$Y \leftarrow U/q_m$
$X \leftarrow (1-Y)(p_- + \lambda_-) + Y(p_+ - \lambda_+)$
if $V \le f(X)/f(p_m)$ **then**
done
end if
else if $U \le q_m + q_+$ **then**
$E \leftarrow -\log\left(\frac{U-q_m}{q_+}\right)$
$X \leftarrow p_+ - \lambda_+(1-E)$
if $V \le e^E f(X)/f(p_m)$ **then**
done
end if
else
$E \leftarrow -\log\left(\frac{U-(q_m+q_+)}{q_-}\right)$
$X \leftarrow p_- + \lambda_-(1-E)$
if $V \le e^E f(X)/f(p_m)$ **then**
done
end if
end if
until done
return X

Require: p_m is the mode of f
p_+ and p_- satisfy $f(p_\pm) = f(p_m)/e$
$\lambda_+ \leftarrow -f(p_+)/f'(p_+)$, $\lambda_- \leftarrow f(p_-)/f'(p_-)$ {can be re-written in terms of $(\log f)'$}
$q_- \leftarrow \frac{\lambda_-}{p_+ - p_-}$, $q_+ \leftarrow \frac{\lambda_+}{p_+ - p_-}$, $q_m \leftarrow 1 - (q_+ + q_-)$
repeat
generate U and V, uniform variates on $[0, 1]$
if $U \le q_m$ **then**
$Y \leftarrow U/q_m$
$X \leftarrow (1-Y)(p_- + \lambda_-) + Y(p_+ - \lambda_+)$
if $V \le f(X)/f(p_m)$ **then**
done
end if
else if $U \le q_m + q_+$ **then**
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$X \leftarrow p_+ - \lambda_+(1-E)$
if $V \le e^E f(X)/f(p_m)$ **then**
done
end if
else
$E \leftarrow -\log\left(\frac{U-(q_m+q_+)}{q_-}\right)$
$X \leftarrow p_- + \lambda_-(1-E)$
if $V \le e^E f(X)/f(p_m)$ **then**
done
end if
end if
until done
return X

Swisdak 2013