SM23A-2766

Loading loss-cone, kappa, and flattop distributions in particle simulations

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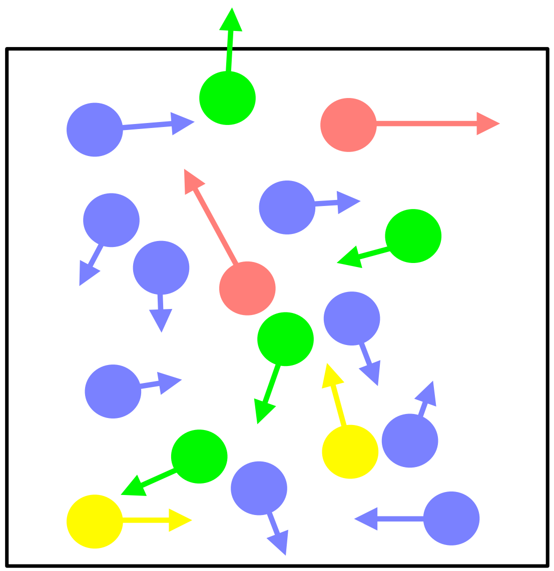
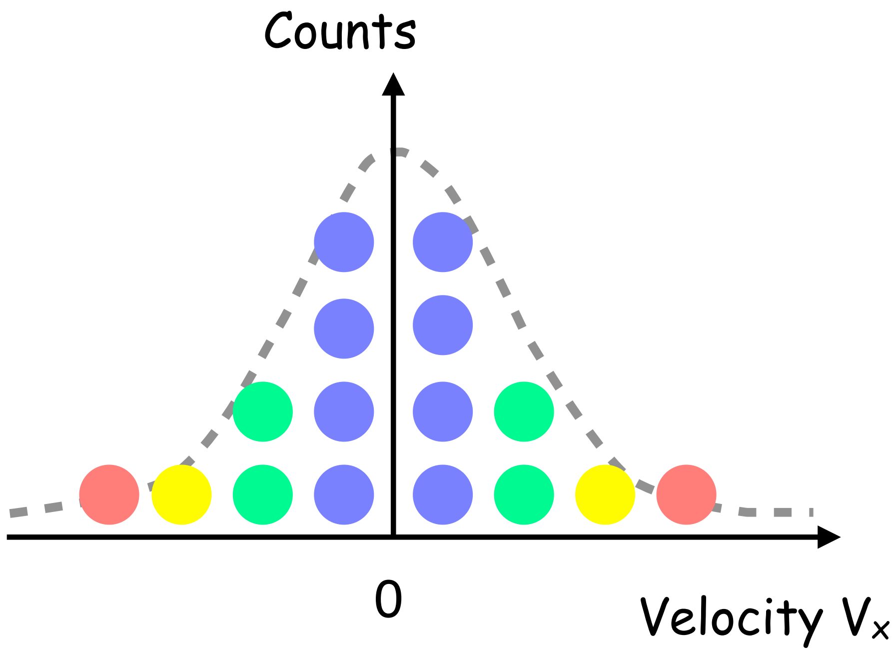
Particle-in-cell (PIC) simulation

- It is very important to randomly prepare <u>velocity distributions</u> of particles in a cell





1. Maxwell distribution

$$f_{\mathrm{M}}(\boldsymbol{v})d^3v = N_M \left(\frac{1}{\pi v_M^2}\right)^{\frac{3}{2}} \exp\left(-\frac{\boldsymbol{v}^2}{v_M^2}\right) d^3v$$

- Normal distribution
  - Box=Muller (1958) method
    - Two random variates: U_1, $U_2 \subset (0,1)$

$$n_1 \leftarrow \sqrt{-2\ln U_1}\cos 2\pi U_2$$

$$n_2 \leftarrow \sqrt{-2\ln U_1}\sin 2\pi U_2$$

How to initialize various velocity distributions
(loss-cone, kappa, flattop...)
in particle-in-cell (PIC) simulation?

1. Maxwell distribution

$$f_{\mathrm{M}}(\boldsymbol{v})d^3v = N_M \left(\frac{1}{\pi v_M^2}\right)^{\frac{3}{2}} \exp\left(-\frac{\boldsymbol{v}^2}{v_M^2}\right) d^3v$$

- Normal distribution
  - Box=Muller (1958) method
    - Two random variates: U_1, U_2 ⊂ [0,1]

$$n_1 \leftarrow \sqrt{-2\ln U_1}\cos 2\pi U_2$$

$$n_2 \leftarrow \sqrt{-2\ln U_1}\sin 2\pi U_2$$

- Spherical form (d^3v --> $4\pi v^2 dv$)

$$f_{\mathrm{M}}(v)dv = 4\pi N_M \left(\frac{1}{\pi v_M^2}\right)^{\frac{3}{2}} \exp\left(-\frac{v^2}{v_M^2}\right) v^2 dv$$

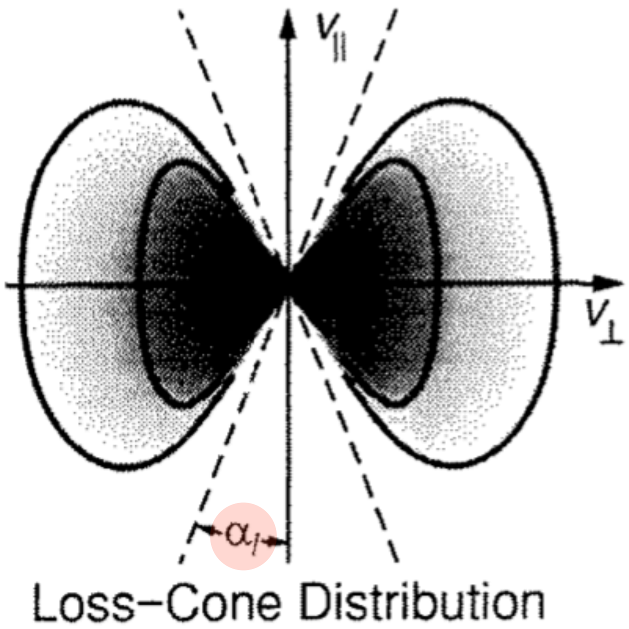
$$f_{\mathrm{M}}(x)dx = \frac{2N_M}{\sqrt{\pi}} x^{1/2} e^{-x} dx = N_M \mathrm{Ga}\left(x; \frac{3}{2}, 1\right) dx$$

Gamma distribution

$$\mathrm{Ga}(x;\alpha,1) = \frac{x^{\alpha-1}e^{-x}}{\Gamma(\alpha)}$$

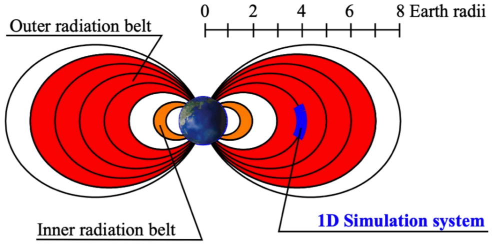
Gamma function

2. Loss-cone distribution - Pitch-angle type



$$\propto \left(\sin \alpha \right)^{2j}$$

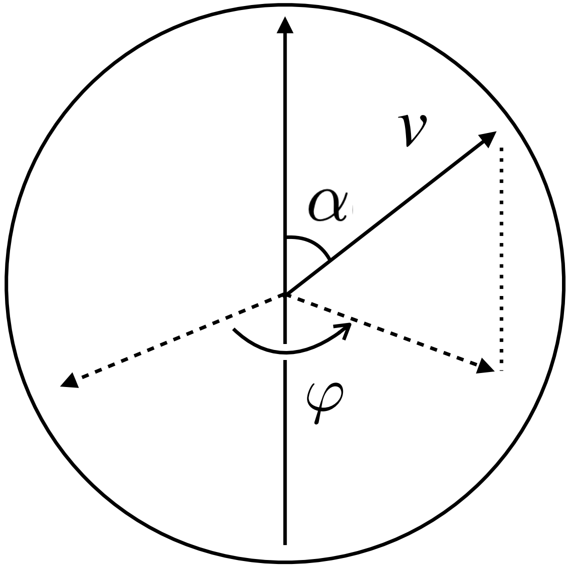
$$\Leftrightarrow \quad \propto \left(\frac{v_\perp}{v} \right)^{2j}$$



(from Katoh-san)

c.f. Kennel 1966

Utilizing Beta distribution



$$\iiint f_0(v)\ (\sin\alpha)^{2j}\, d^3v$$

$$= 4\pi\left(\int_0^\infty v^2 f_0(v)\, dv\right)\left(\int_0^{\pi/2} (\sin\alpha)^{2j+1}\, d\alpha\right)$$

$$x \equiv \cos^2\alpha$$

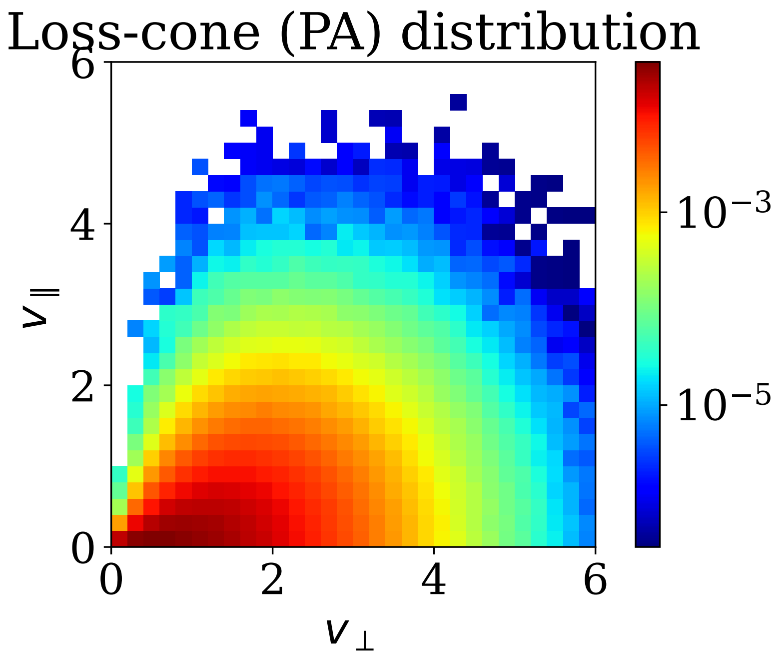
$$\longrightarrow \frac{B(1/2, j+1)}{2}\left\{\int_0^1 \frac{(1-x)^j x^{-1/2}}{B(1/2, j+1)} dx\right\}$$

Beta function

Beta distribution

- One can transform isotropic distributions to loss-cone distributions via Beta random variate.
- Beta variate can be generated from two gamma variates

Loss-cone distribution - Recipe



Algorithm 5.3: Loss-cone distribution

generate $N \sim \mathcal{N}(0, 1)$

generate $X_1 \sim \mathrm{Ga}(3/2, 1)$

generate $X_2 \sim \mathrm{Ga}(j + 1, 2)$

generate $U \sim U(0, 1)$

$v_{\perp 1} \leftarrow \theta \sqrt{X_1} \sqrt{\frac{X_2}{N^2 + X_2}} \cos(2\pi U)$

$v_{\perp 2} \leftarrow \theta \sqrt{X_1} \sqrt{\frac{X_2}{N^2 + X_2}} \sin(2\pi U)$

$v_\parallel \leftarrow \theta \sqrt{X_1} \frac{N}{\sqrt{N^2 + X_2}}$

return $v_{\perp 1}, v_{\perp 2}, v_\parallel$

Loss-cone transform (Beta variate)

$$f(\boldsymbol{v}) = \frac{N_0}{\pi^2 \theta^3} \frac{2\Gamma(j + 3/2)}{\Gamma(j + 1)} \left(\frac{v_\perp}{v} \right)^{2j} \exp\left(- \frac{v^2}{\theta^2} \right)$$

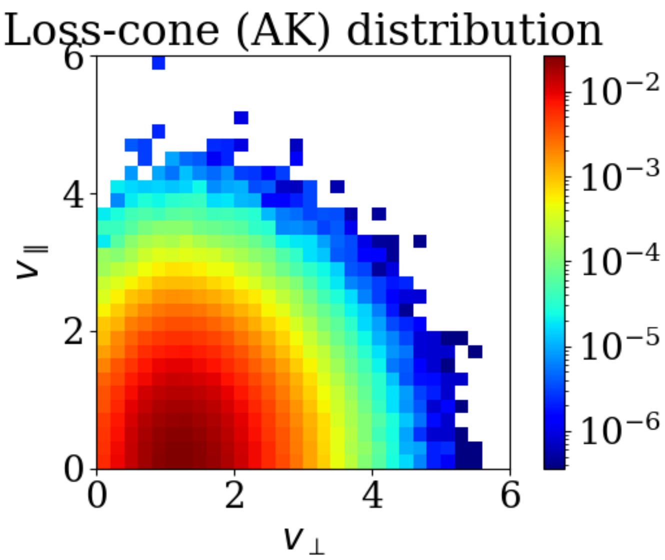
2. Loss-cone distributions - Subtracted Maxwellian

[Ashour-Abdalla & Kennel, 1978]

$$f(v_\parallel, v_\perp) = \frac{N_0}{\pi^{1/2}\theta_\parallel} \exp\left(-\frac{v_\parallel^2}{\theta_\parallel^2}\right) \times \frac{1}{\pi\theta_\perp^2} \left\{\Delta \exp\left(-\frac{v_\perp^2}{\theta_\perp^2}\right) + \frac{1-\Delta}{1-\beta}\left[\exp\left(-\frac{v_\perp^2}{\theta_\perp^2}\right) - \exp\left(-\frac{v_\perp^2}{\beta\theta_\perp^2}\right)\right]\right\}$$

Loss-cone filling factor Δ

Shape factor β



Algorithm 2*

generate $U_1, U_2, U_3 \sim U(0,1)$

generate $N \sim \mathcal{N}(0,1)$

$x \leftarrow -\log U_1 - \beta \log\left(\min\left(\frac{U_2}{1-\Delta}, 1\right)\right)$

$v_{\perp 1} \leftarrow \theta_\perp \sqrt{x} \cos(2\pi U_3)$

$v_{\perp 2} \leftarrow \theta_\perp \sqrt{x} \sin(2\pi U_3)$

$v_\parallel \leftarrow \theta_\parallel \sqrt{1/2}\, N$

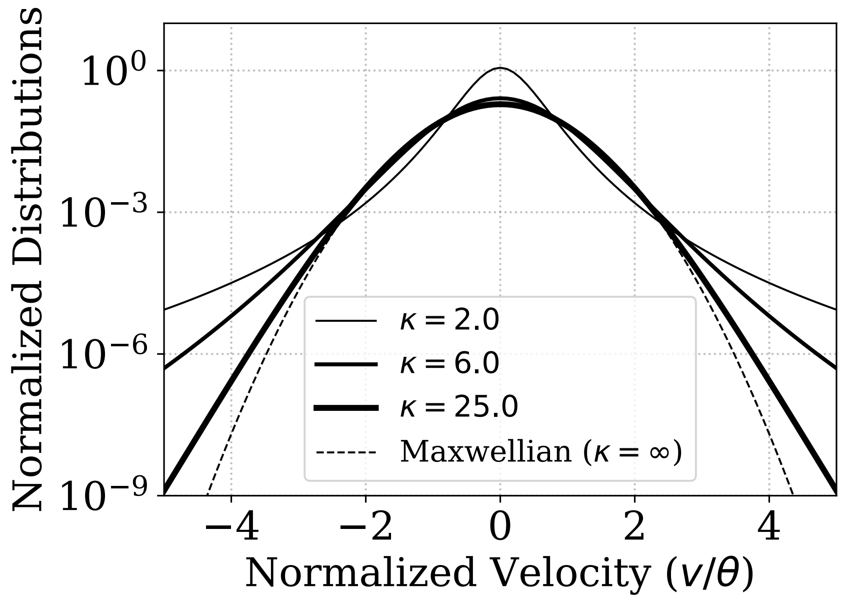
return $v_{\perp 1}, v_{\perp 2}, v_\parallel$

3. Kappa distribution

$$f(\boldsymbol{v})d^3v = \frac{N}{(\pi\kappa\theta^2)^{3/2}} \frac{\Gamma(\kappa+1)}{\Gamma(\kappa-1/2)} \left(1 + \frac{v^2}{\kappa\theta^2}\right)^{-(\kappa+1)} d^3v$$

- Thermal core + power-law tail
- Popular in space physics (Vasyliunas 1968, Olbert 1968)

- κ : power-law index
- κ --> ∞ Maxwellian



3. Kappa distribution

- Spherical form

$$f_\kappa(v)dv = N_\kappa \frac{4}{\pi^{1/2}(\kappa\theta^2)^{3/2}} \frac{\Gamma(\kappa+1)}{\Gamma(\kappa-1/2)} \left(1+\frac{v^2}{\kappa\theta^2}\right)^{-(\kappa+1)} v^2 dv$$

$$= N_\kappa \mathrm{B}'\left(v; \frac{3}{2}, \frac{\nu}{2}, 2, (\kappa\theta^2)^{1/2}\right) dv.$$

- Generalized Beta-prime distribution

$$\mathrm{B}'(x;\alpha,\beta,p,q) = \frac{p}{qB(\alpha,\beta)} \left(\frac{x}{q}\right)^{\alpha p-1} \left(1+\left(\frac{x}{q}\right)^p\right)^{-(\alpha+\beta)}$$

- Beta-prime random number

Gamma random number

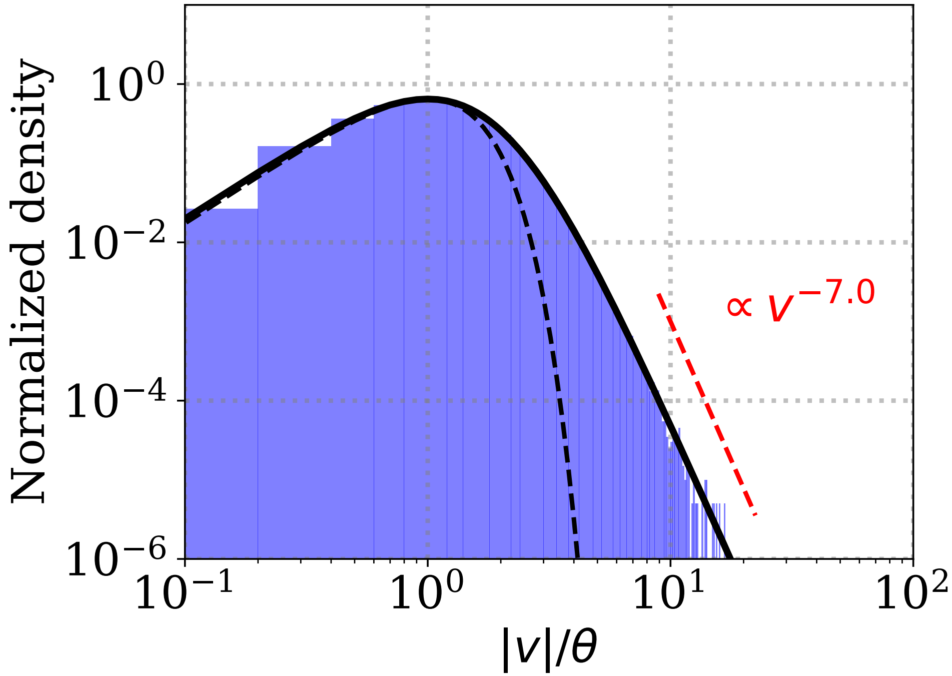
$$X_{\mathrm{B}'(\alpha,\beta,p,q)} = q\left(\frac{X_{\mathrm{Ga}(\alpha,\delta)}}{X_{\mathrm{Ga}(\beta,\delta)}}\right)^{1/p}$$

Gamma random number

(Kappa distribution) $= \sqrt{\kappa\theta^2}$ $\dfrac{\text{(Normal distribution)}}{\sqrt{X_{Ga(\kappa-1/2,2)}}}$

3. Kappa distribution - Recipe

$$f(\boldsymbol{v})d^3v = \frac{N}{(\pi\kappa\theta^2)^{3/2}}\frac{\Gamma(\kappa+1)}{\Gamma(\kappa-1/2)}\left(1+\frac{v^2}{\kappa\theta^2}\right)^{-(\kappa+1)}d^3v$$



Algorithm 1-2

generate $n_1, n_2, n_3 \sim \mathcal{N}(0,1)$

generate $\chi^2_\nu \sim \mathrm{Ga}(\kappa - 1/2, 2)$

$r \leftarrow \sqrt{\dfrac{\kappa\theta^2}{\chi^2_\nu}}$

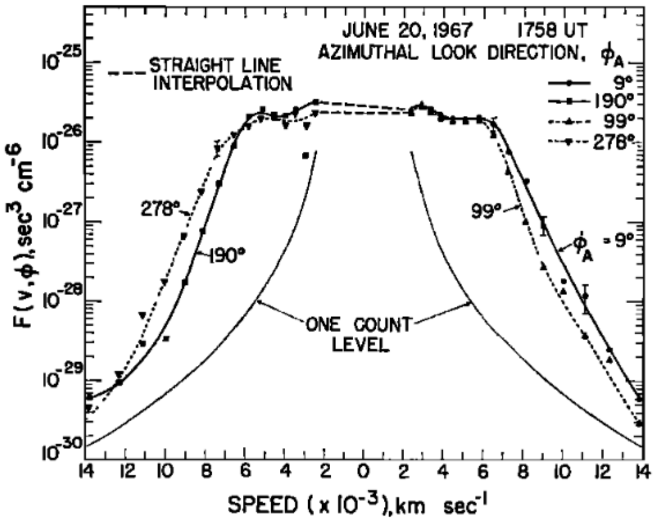
$v_x \leftarrow r n_1$

$v_y \leftarrow r n_2$

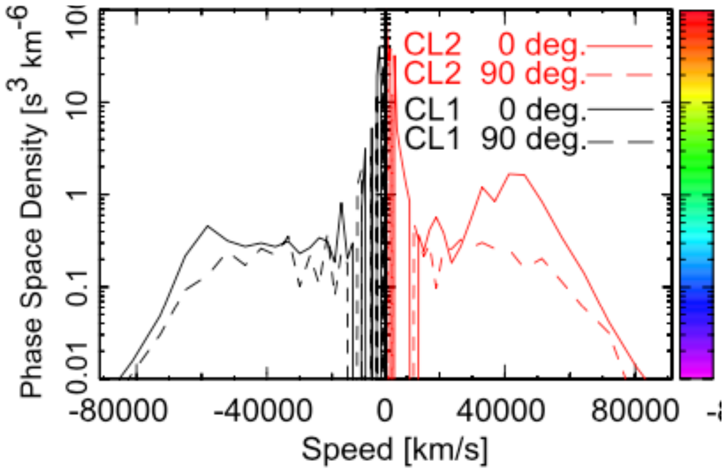
$v_z \leftarrow r n_3$

See also Abdul & Mace 2015

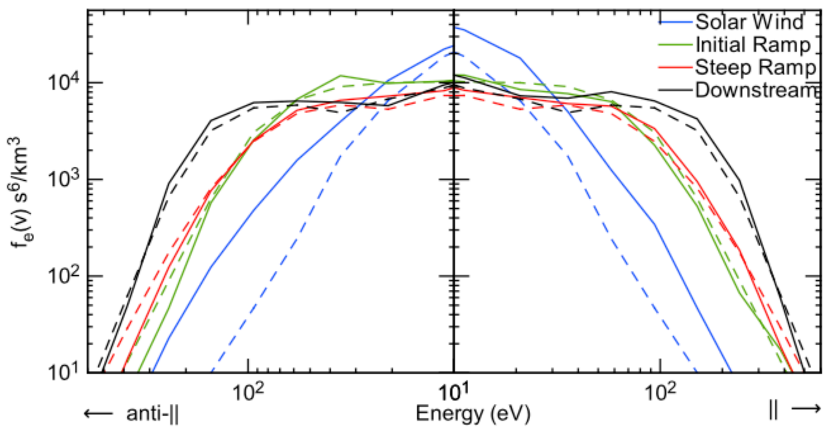
4. Flattop (FT) distribution



Montgomery+ 1970 JGR



Asano+ 2008 JGR



Schwartz+ 2011 PRL

- Shocked magnetosheath
- Magnetic reconnection

4. Flattop (FT) distribution

- Popular kappa-like form (Thomsen+ 1983, Oka+ 2022)
  - Other forms are also discussed (Wilson+ 2019)

$$f_{\rm ft}(\vec{v})d^3v = \frac{3N_{\rm ft}}{4\pi(\theta_{\parallel}\theta_{\perp}^2)} \frac{\Gamma\left(1+\dfrac{1}{\kappa}\right)}{\Gamma\left(1+\dfrac{3}{2\kappa}\right)\Gamma\left(1-\dfrac{1}{2\kappa}\right)} \left(1+\left(\frac{v_{\parallel}^2}{\theta_{\parallel}^2}+\frac{v_{\perp}^2}{\theta_{\perp}^2}\right)^{\kappa}\right)^{-(\kappa+1)/\kappa} d^3v$$

- Generalized beta-prime distribution

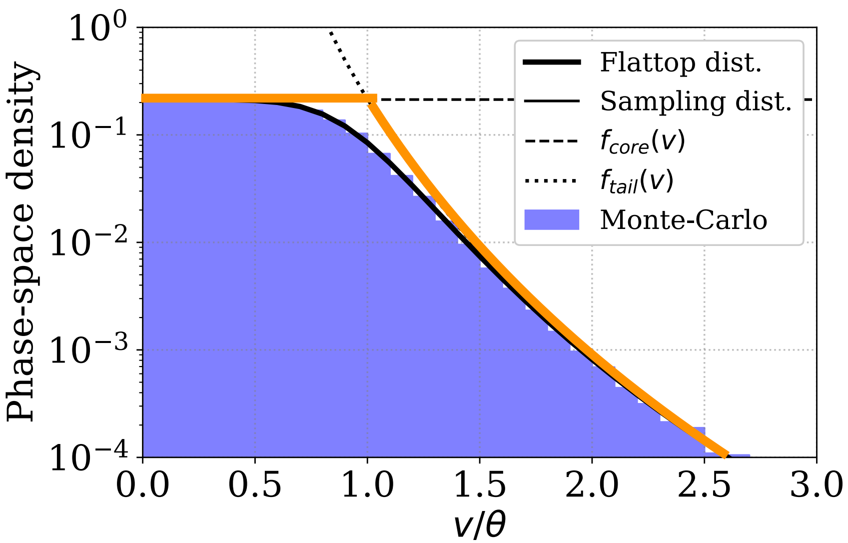
$$\mathrm{B}'(x;\alpha,\beta,p,q) = \frac{\alpha p\,\Gamma(\alpha+\beta)}{q^{\alpha p}\Gamma(1+\alpha)\Gamma(\beta)} \left(1+\left(\frac{x}{q}\right)^{p}\right)^{-(\alpha+\beta)} x^{\alpha p-1}$$

- FT distribution in spherical coordinates

$$F_{\rm ft}(v) \equiv f_{\rm ft}(v)4\pi v^2 = \frac{3N}{\theta^3} \frac{\Gamma\left(1+\frac{1}{\kappa}\right)}{\Gamma\left(1+\frac{3}{2\kappa}\right)\Gamma\left(1-\frac{1}{2\kappa}\right)} \left(1+\left(\frac{v}{\theta}\right)^{2\kappa}\right)^{-(\kappa+1)/\kappa} v^2$$

$$= NB'\left(v;\frac{3}{2\kappa},1-\frac{1}{2\kappa},2\kappa,\theta\right)$$

Flattop (FT) - Piecewise rejection method



$p_1 \leftarrow \frac{2\kappa - 1}{2\kappa + 2}$, $p_2 \leftarrow \frac{3}{2\kappa + 2}$

repeat

generate $X_1, X_2 \sim U(0,1)$

if $X_1 \leq p_1$ **then**

$x \leftarrow (X_1/p_1)^{1/3}$

if $X_2 < (1 + x^{2\kappa})^{-(\kappa+1)/\kappa}$, **break**

else

$x \leftarrow ((1 - X_1)/p_2)^{1/(1-2\kappa)}$

if $X_2 < (x^{-2\kappa} + 1)^{-(\kappa+1)/\kappa}$, **break**

endif

end repeat

generate $X_3, X_4 \sim U(0,1)$

$v_{\perp 1} \leftarrow 2\theta_\perp x \sqrt{X_3(1 - X_3)} \cos(2\pi X_4)$

$v_{\perp 2} \leftarrow 2\theta_\perp x \sqrt{X_3(1 - X_3)} \sin(2\pi X_4)$

$v_\parallel \leftarrow \theta_\parallel x \ (2X_3 - 1)$

return $v_{\perp 1}, v_{\perp 2}, v_\parallel$

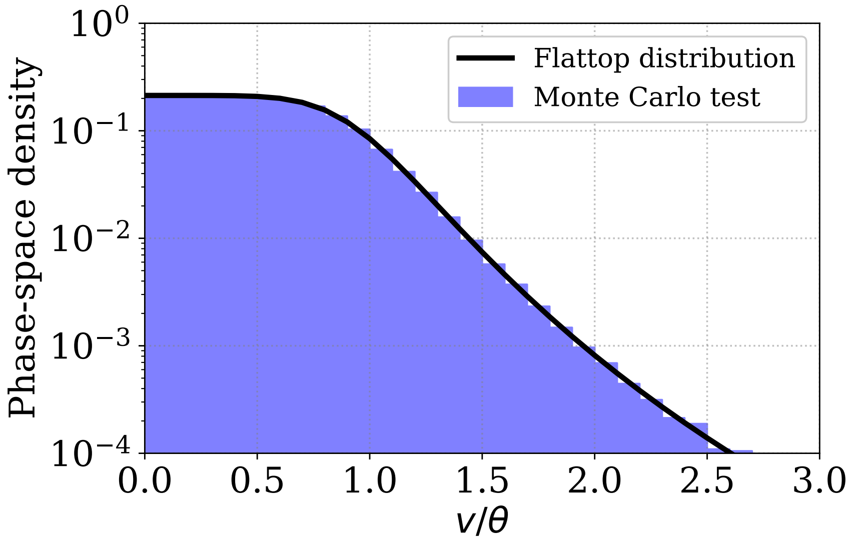
- Envelope: flat core & tail
- Acceptance efficiency: 60%~
- Can we make it more efficiently?

Flattop (FT) - Gamma method

- Beta-prime random number

$$X_{\mathrm{B}'(\alpha,\beta,p,q)} = q\left(X_{\mathrm{B}'(\alpha,\beta)}\right)^{1/p} = q\left(\frac{X_{\mathrm{Ga}(\alpha,\delta)}}{X_{\mathrm{Ga}(\beta,\delta)}}\right)^{1/p}$$

Gamma random numbers

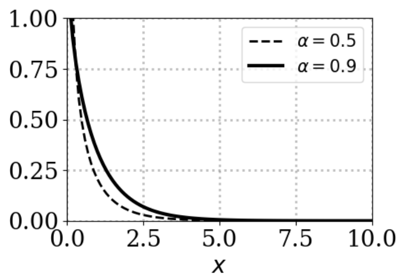


$$\begin{aligned}
&\text{generate } X_1 \sim \mathrm{Gamma}(3/(2\kappa), 1)\\
&\text{generate } X_2 \sim \mathrm{Gamma}(1 - 1/(2\kappa), 1)\\
&\text{generate } X_3, X_4 \sim U(0,1)\\
&v \;\; \leftarrow (X_1/X_2)^{1/(2\kappa)}\\
&v_{\parallel} \;\; \leftarrow \;\; \theta_{\parallel} v \;(2X_3 - 1)\\
&v_{\perp 1} \leftarrow 2\theta_{\perp} v \sqrt{X_3(1-X_3)}\cos(2\pi X_4)\\
&v_{\perp 2} \leftarrow 2\theta_{\perp} v \sqrt{X_3(1-X_3)}\sin(2\pi X_4)
\end{aligned}$$

- Acceptance efficiency is not 100%, because...

5. Gamma-distributed random number

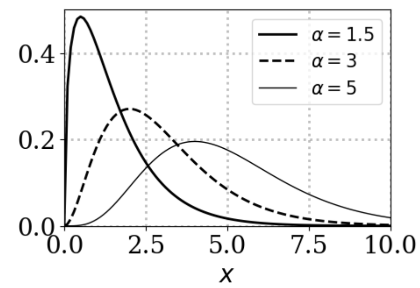
α<1

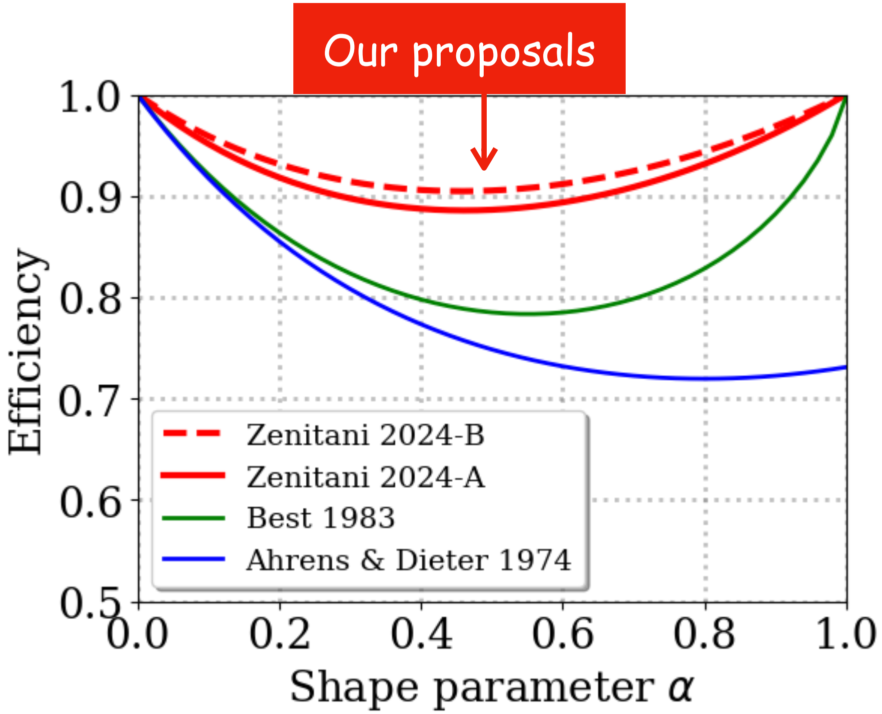


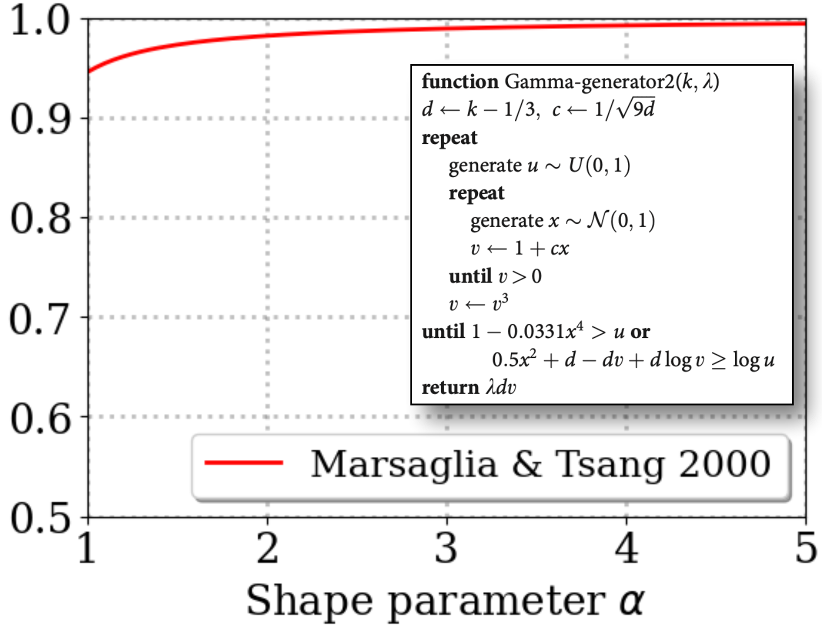
α: Shape parameter

$$\mathrm{Ga}(x;\alpha,1)=\frac{x^{\alpha-1}e^{-x}}{\Gamma(\alpha)}$$

1<α







New gamma generator

[Zenitani 2024, Econ. Bull.]

- Generalized exponential function (Kundu & Gupta 2007)

$$F_{\exp}(x;\alpha) = (1 - e^{-x})^{\alpha}$$

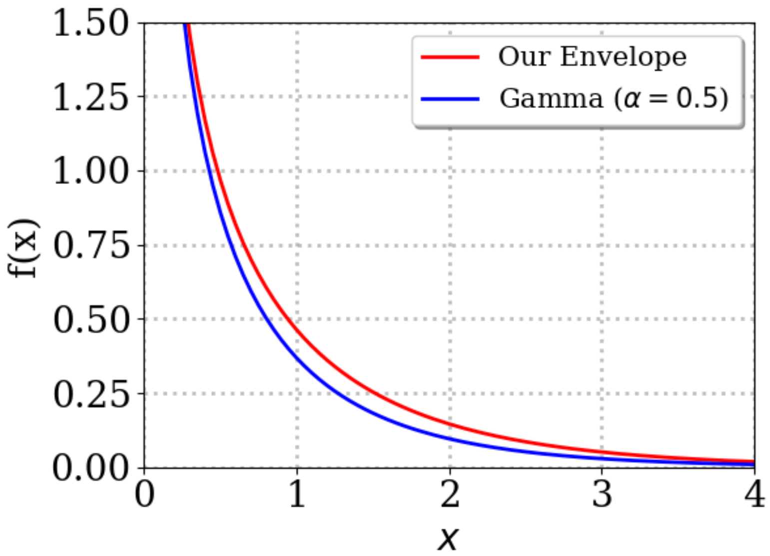
- Its derivative

$$f_{\exp}(x;\alpha) = \alpha(1 - e^{-x})^{\alpha-1} e^{-x}$$

↔

Gamma distribution

$$f_{\Gamma}(x;\alpha) = \frac{1}{\Gamma(\alpha)} x^{\alpha-1} e^{-x}$$



Algorithm 1

repeat

generate $U_1, U_2 \sim U(0,1)$

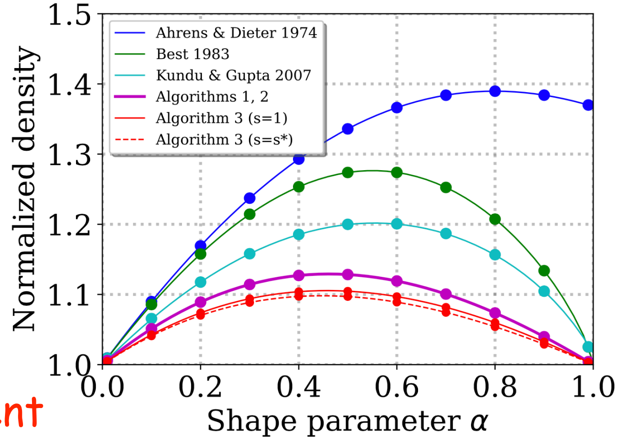
$b \leftarrow U_1^{1/\alpha}$, $x \leftarrow -\log(1-b)$

if $U_2^{1/(1-\alpha)} x \leq b$ **return** x

end repeat

New gamma generator

[Zenitani 2024, Econ. Bull.]



efficient

- A mathematical trick makes our algorithm even faster

$$\frac{4+(\alpha-1)x}{4+(1-\alpha)x} \le \left(\frac{x}{1-e^{-x}}\right)^{\alpha-1} \le \frac{4+\alpha x}{4+(2-\alpha)x}$$

Algorithm 2

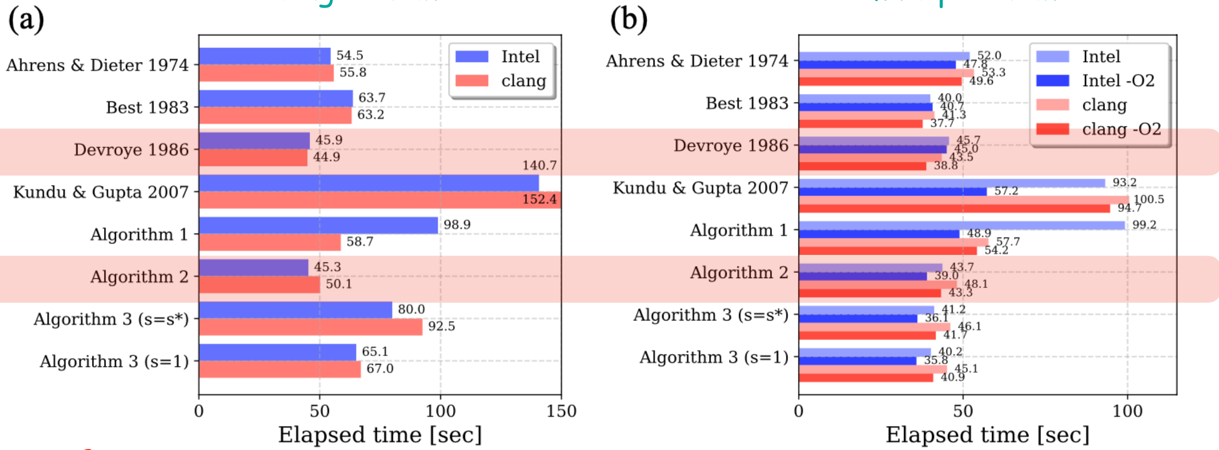
repeat
  generate $U_1, U_2 \sim U(0,1)$
  $b \leftarrow U_1^{1/\alpha}$, $x \leftarrow -\log(1-b)$
  if $U_2(4+(1-\alpha)x) \le (4+(\alpha-1)x)$ **return** x
  if $U_2(4+(2-\alpha)x) \le (4+\alpha x)$ **then**
    if $U_2^{1/(1-\alpha)} x \le b$ **return** x
end repeat

single draw

multiple draw

Devroye 1986 (NumPy) →

Zenitani 2024 →



fast ←

Summary

Numerical recipes consist of

1. uniform variate
2. normal variate
3. gamma variate

- 1. Maxwell distribution
- 2. Loss-cone distribution
    - Beta distribution to scatter
- 3. Kappa distribution
    - Normal distribution, divided by Gamma distribution
- 4. Flattop distribution
    - Piecewise rejection and gamma methods
- 5. Gamma distribution
    - New generator for shape parameter less than unity
- References

- [2] Zenitani & Nakano, *JGR Space Physics*, 128, e2023JA031983 (2023)
- [3] Zenitani & Nakano, *Phys. Plasmas*, 29, 113904 (2022)
- [4] Zenitani, *Research Notes of the AAS*, 8, 30 (2024)
- [5] Zenitani, *Economics Bulletin*, 44, 1113 (2024), arXiv:2411.01415