Loading various velocity distributions in particle-in-cell (PIC) simulation

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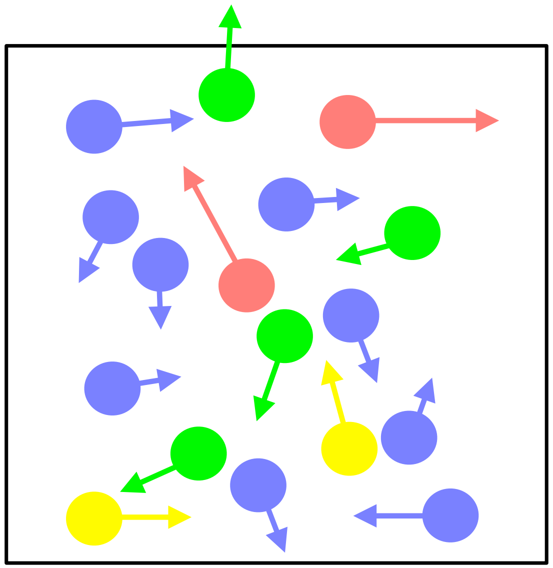
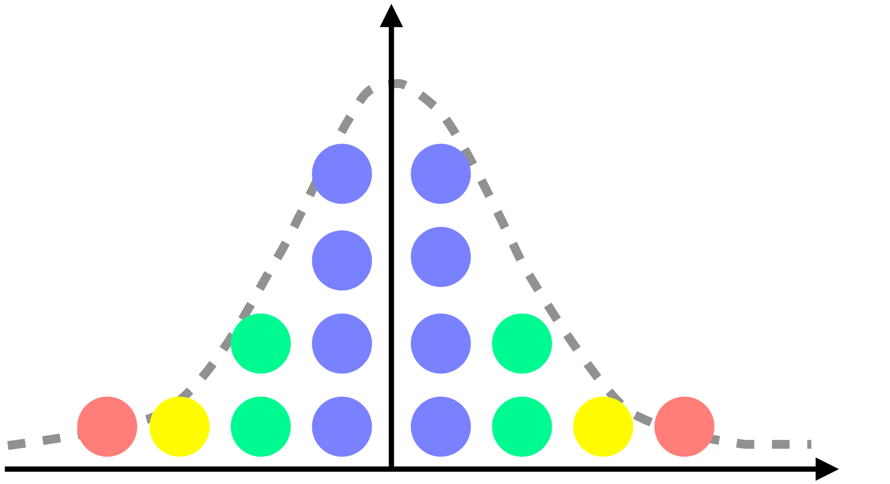
Particle-in-cell (PIC) simulation

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





0. 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 (Kappa, loss-cone, relativistic...) in particle-in-cell (PIC) simulation?

0. Maxwell distribution

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

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

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

Gamma distribution

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

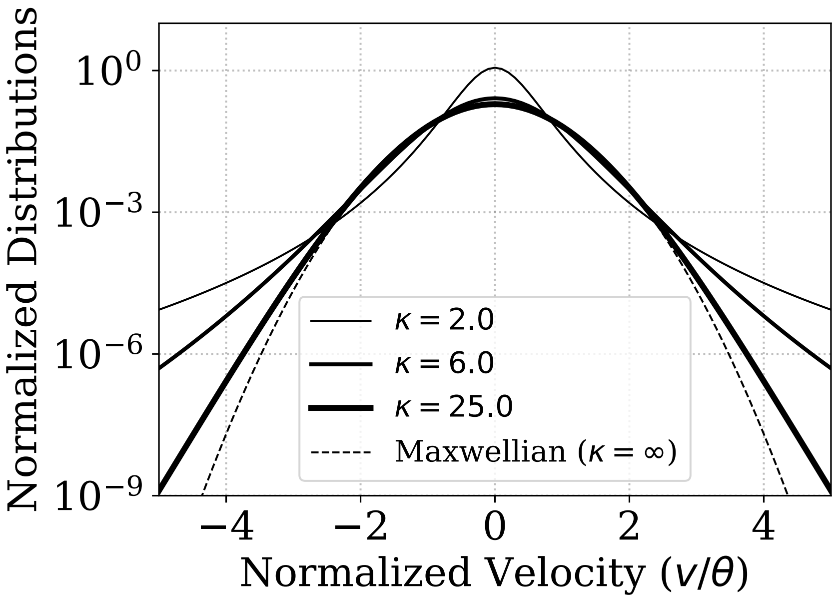
Gamma function

1. 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
- $\kappa \to \infty$ Maxwellian



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

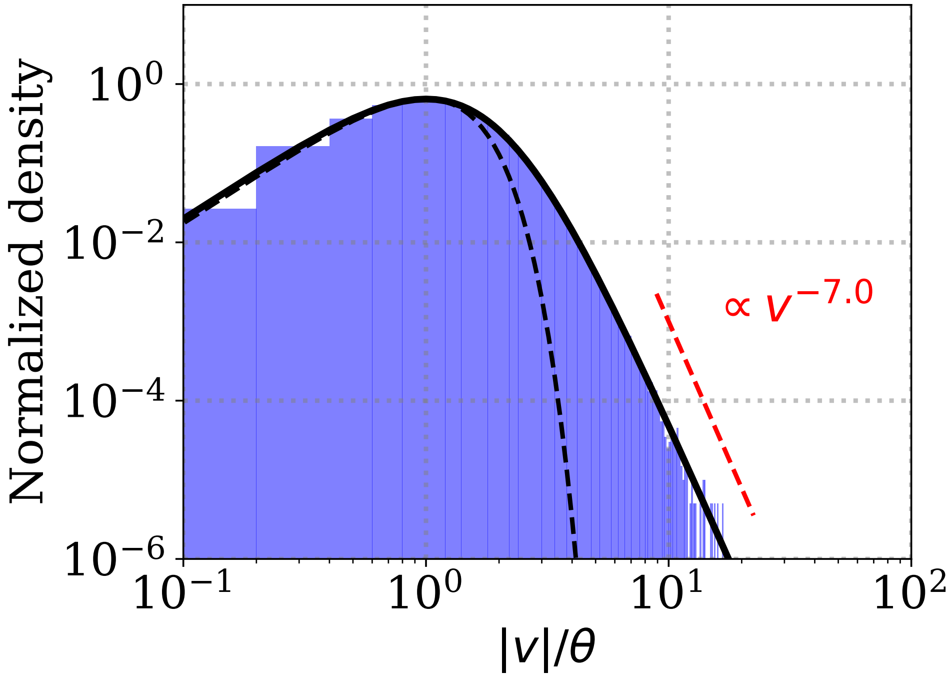
$$X_{\mathrm{B}'(\alpha,\beta,p,q)} = q\left(\frac{X_{\mathrm{Ga}(\alpha,\delta)}}{X_{\mathrm{Ga}(\beta,\delta)}}\right)^{1/p}$$

Gamma random number

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

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

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

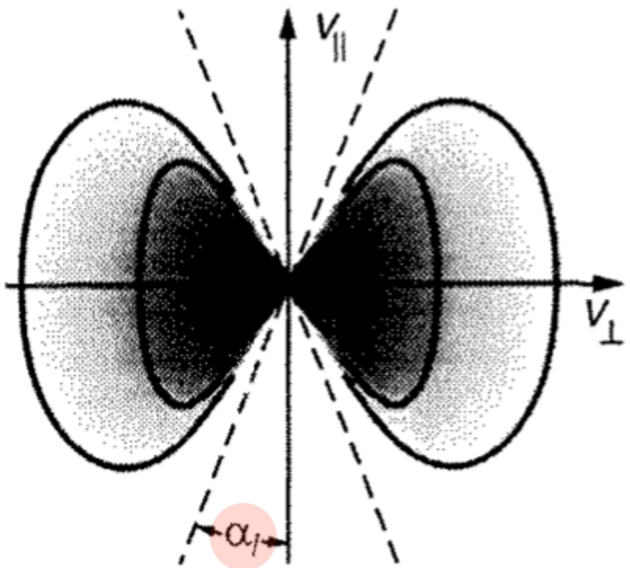
$v_x \leftarrow rn_1$

$v_y \leftarrow rn_2$

$v_z \leftarrow rn_3$

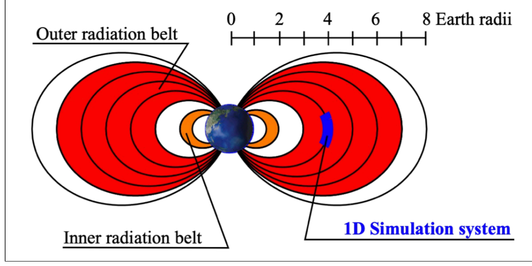
See also Abdul & Mace 2015

2. Loss-cone distribution (Pitch-angle type)



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

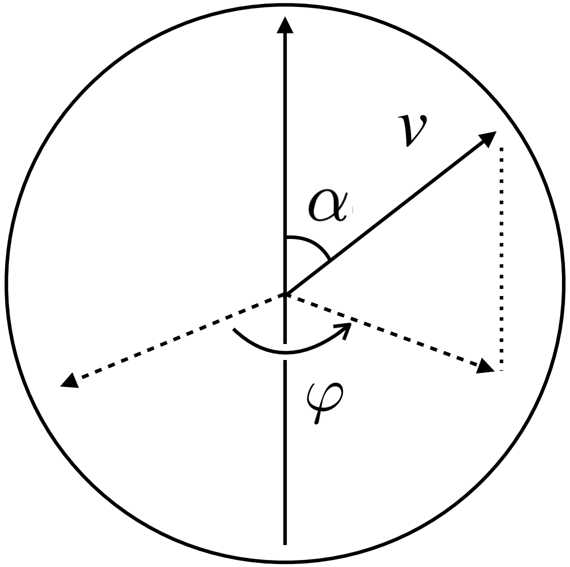
$$\Leftrightarrow \quad \propto \left(\frac{v_\perp}{v} \right)^{2j}$$



(from Katoh-san)

c.f. Kennel 1966

Utilizing Beta distribution



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

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

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

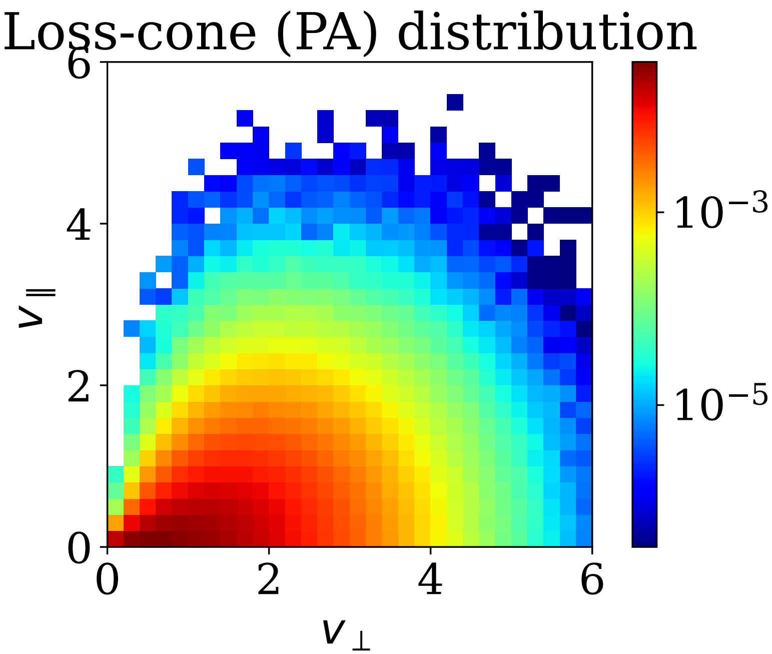
$$\longrightarrow \frac{B(1/2, j+1)}{2}\left\{\int_0^1 \frac{(1-x)^j x^{-1/2}}{B(1/2, j+1)} dx\right\}$$

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)

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

3. Relativistic Maxwell distribution

(Maxwell=Jüttner distribution)

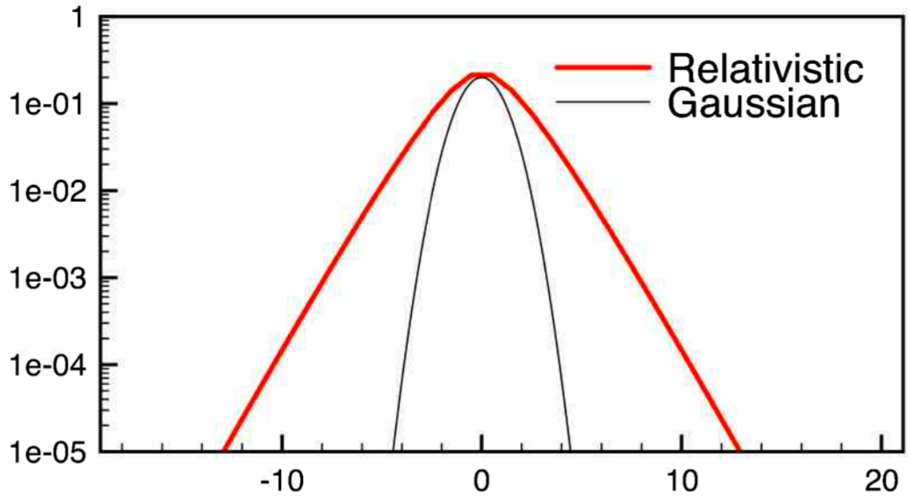
$$f_{\mathrm{MJ}}(\boldsymbol{p})d^3p = \frac{N_M}{4\pi m^2 c T_M K_2(mc^2/T_M)} \exp\left(-\frac{\gamma mc^2}{T_M}\right) d^3p$$

Modified Bessel function of the second kind

Lorentz factor

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

- Lorentz factor makes the distribution complex



$$p_x = \gamma m v_x$$

Modified Canfield method

[Canfield+ 1987, Zenitani & Nakano 2022]

- Spherical form, as a function of the energy

$$f(x)dx = \frac{e^{-1/t}}{tK_2(1/t)} e^{-x/t} \,(1+x)\sqrt{x(x+2)}\; dx \qquad x \equiv \frac{\mathcal{E}_{\rm kin}}{mc^2} = \gamma - 1$$

$$\times \frac{\sqrt{2} + ax^{1/2} + b\sqrt{2}x + x^{3/2}}{\sqrt{2} + ax^{1/2} + b\sqrt{2}x + x^{3/2}} \qquad (a,b) = (0.56, 0.35)$$

$$f(x)dx = \frac{\sqrt{t}e^{-1/t}S(t)}{\sqrt{2}K_2(1/t)} \left(\sum_{i=3}^{6} \pi_i(t)\, Ga\left(x; \frac{i}{2}, t\right) \right) R(x)\; dx$$

Probability

$$\sum_{i=3}^{6} \pi_i(t) = 1$$

Gamma distribution

$$Ga(x; k, \lambda) = \frac{1}{\lambda^k \Gamma(k)} x^{k-1} e^{-x/\lambda}$$

Rejection function (0.95 < R < 1.0)

$$R(x; a, b) \equiv \frac{(1+x)\sqrt{x+2}}{\sqrt{2} + ax^{1/2} + b\sqrt{2}x + x^{3/2}}$$

Modified Canfield method - Recipe

compute π_3, π_4, π_5 for given t using Eqs. (69)–(71)

repeat

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

  if $X_1 < \pi_3$ **then** $i \leftarrow 3$

  elseif $X_1 < \pi_3 + \pi_4$ **then** $i \leftarrow 4$

  elseif $X_1 < \pi_3 + \pi_4 + \pi_5$ **then** $i \leftarrow 5$

  else $i \leftarrow 6$

  endif

  generate $x \sim \mathrm{Ga}(i/2, t)$ — Gamma distribution

until $X_2 < 0.95$ **or** $X_2 < R(x)$ — Rejection

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

$p \leftarrow \sqrt{x\,(x+2)}$

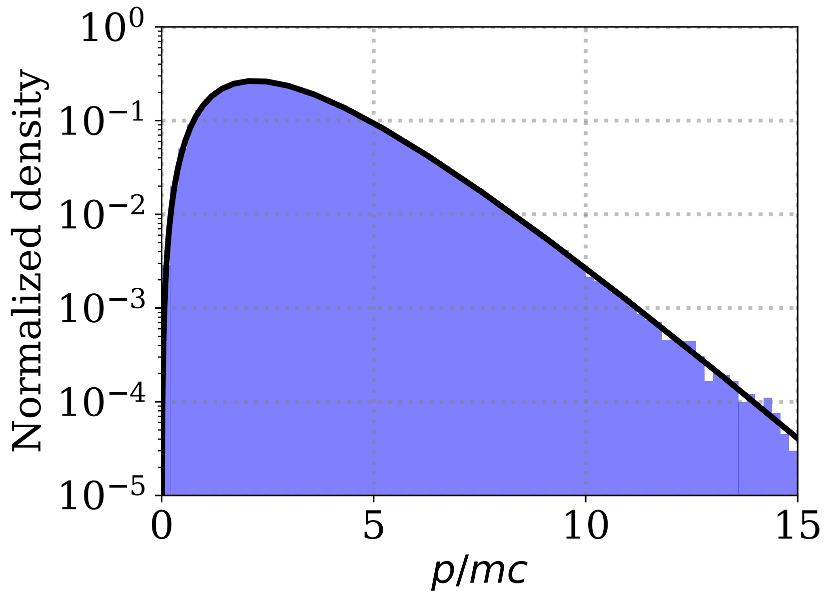
$p_x \leftarrow p\,(2X_3 - 1)$

$p_y \leftarrow 2p\sqrt{X_3(1-X_3)}\cos(2\pi X_4)$

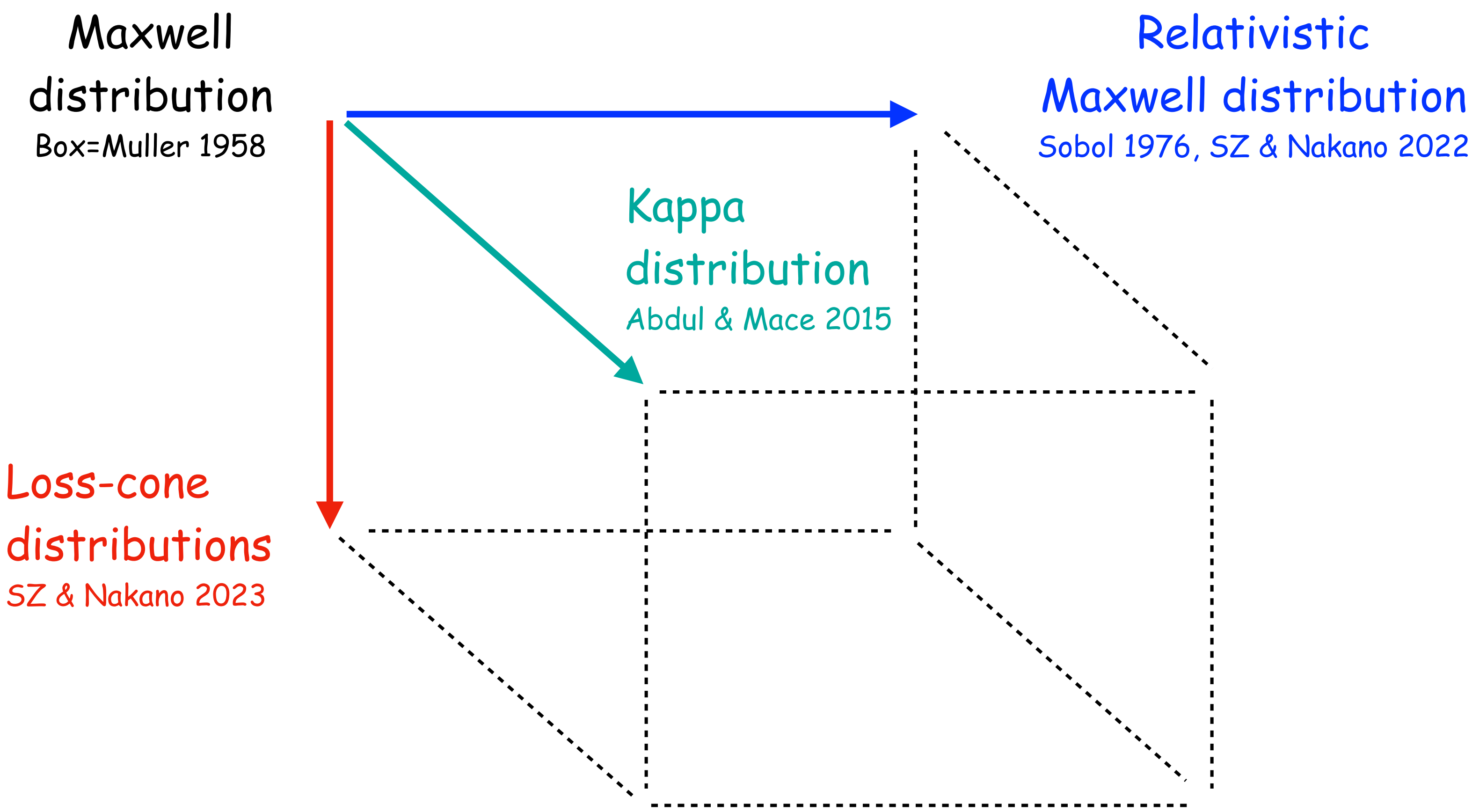
$p_z \leftarrow 2p\sqrt{X_3(1-X_3)}\sin(2\pi X_4)$

return p_x, p_y, p_z

- Gamma-distributed variates are necessary
- Rejection : acceptance efficiency is 95.7-100%.



Velocity distributions



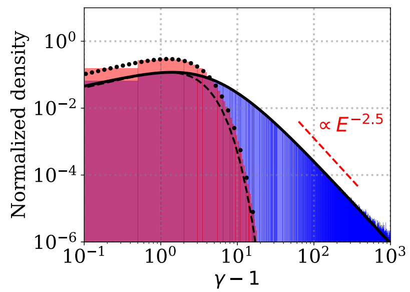
Velocity distributions

Maxwell distribution
Box=Muller 1958

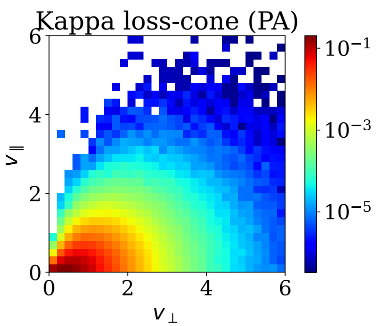
Relativistic Maxwell distribution
Sobol 1976, SZ & Nakano 2022

Kappa distribution
Abdul & Mace 2015

Relativistic kappa distribution
SZ & Nakano 2022



Loss-cone distributions
SZ & Nakano 2023



Kappa loss-cone (KLC) distributions

Velocity distributions

Maxwell distribution
Box=Muller 1958

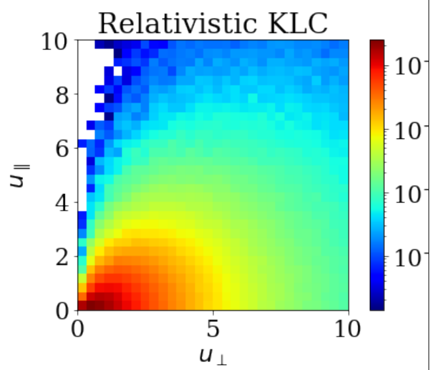
Relativistic Maxwell distribution
Sobol 1976, SZ & Nakano 2022

Kappa distribution
Abdul & Mace 2015

Relativistic kappa distribution
SZ & Nakano 2022

Loss-cone distributions
SZ & Nakano 2023

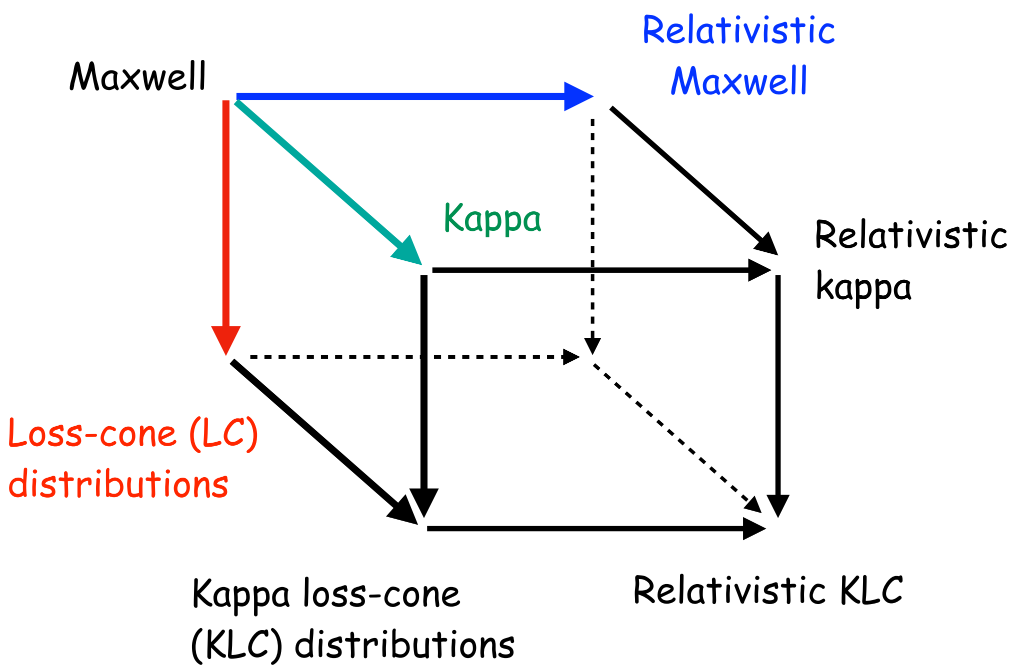
Relativistic loss-cone distribution

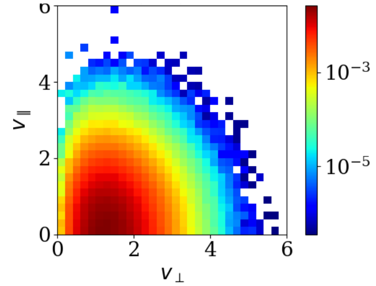


Kappa loss-cone (KLC) distributions

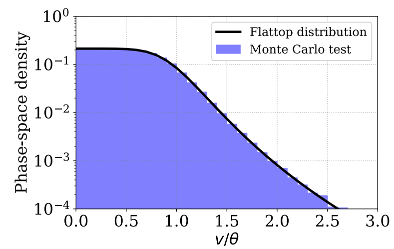
Relativistic kappa loss-cone (KLC) distribution

Various distributions





- Subtracted Maxwellian
- Dory
- Summers KLC
- Flattop
- Flattop losscone



- Numerical recipes require
  - Uniform random number
  - Normal random number
  - Gamma random number

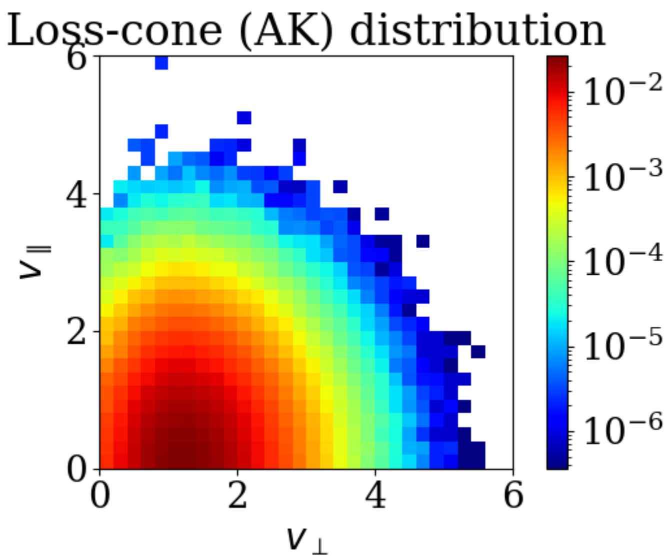
Subtracted Maxwellian

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

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

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

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

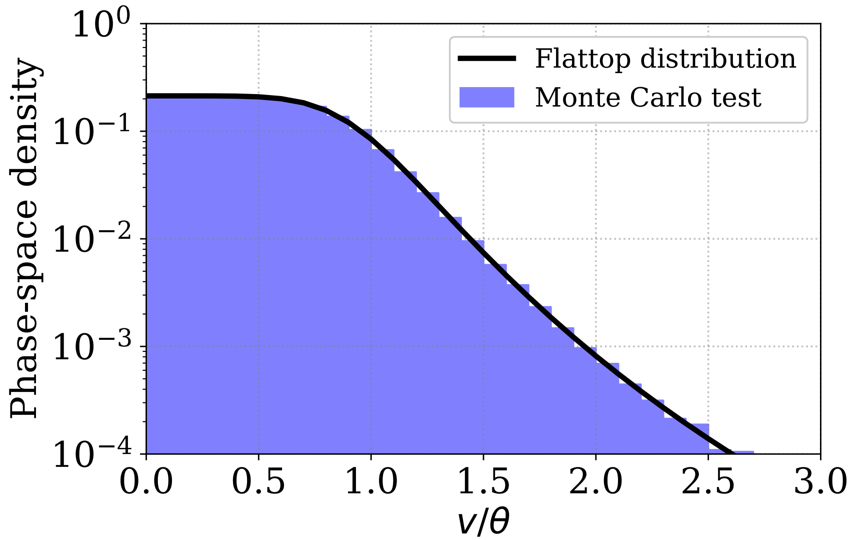
$v_\parallel \leftarrow \theta_\parallel \sqrt{1/2}\, N$

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

Flattop distribution

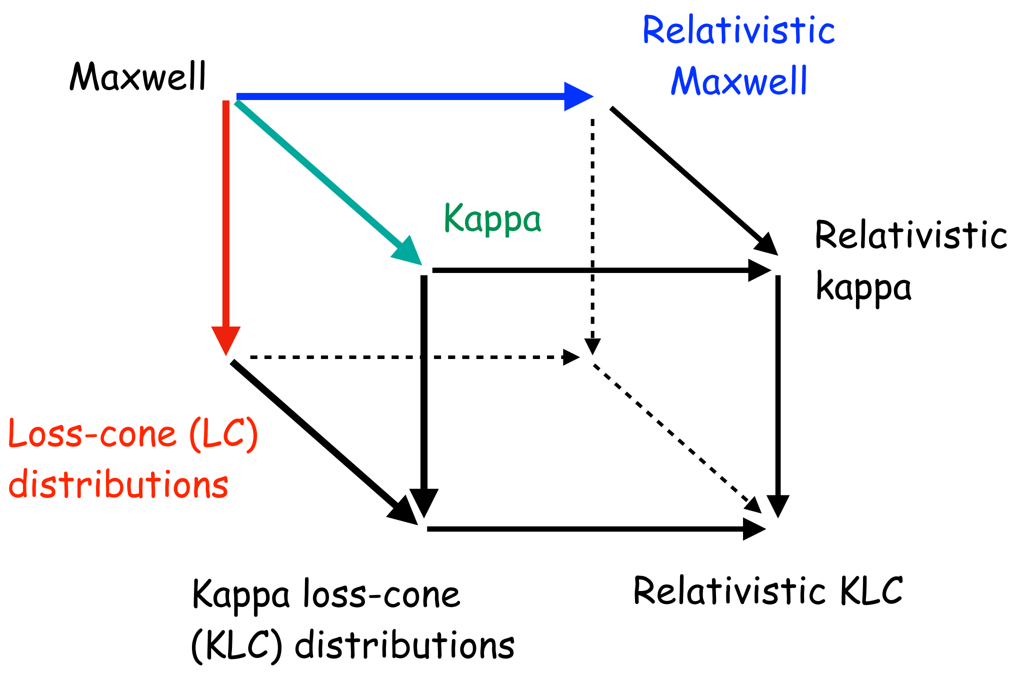
[Zenitani 2024 RNAAS]

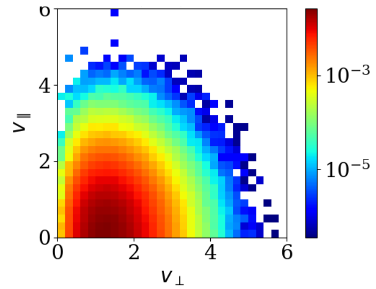
$$f_{\rm ft}(\vec{v})d^3v = \frac{3N_{\rm ft}}{4\pi(\theta_{\|}\theta_{\perp}^2)} \frac{\Gamma\left(1+\frac{1}{\kappa}\right)}{\Gamma\left(1+\frac{3}{2\kappa}\right)\Gamma\left(1-\frac{1}{2\kappa}\right)} \left(1+\left(\frac{v_{\|}^2}{\theta_{\|}^2}+\frac{v_{\perp}^2}{\theta_{\perp}^2}\right)^{\kappa}\right)^{-(\kappa+1)/\kappa}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



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

Various distributions





- Subtracted Maxwellian
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- Summers KLC
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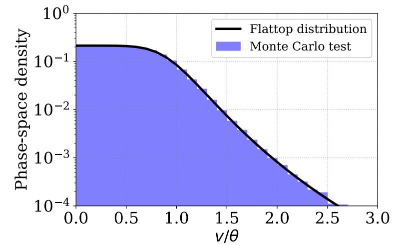
- Flattop losscone

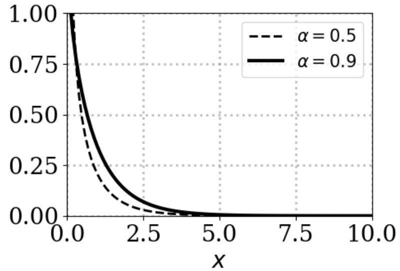


- Numerical recipes require
  - Uniform random number
  - Normal random number
  - Gamma random number

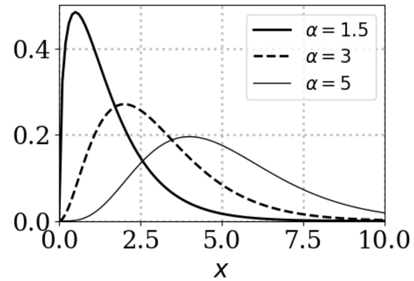
Gamma-distributed random number

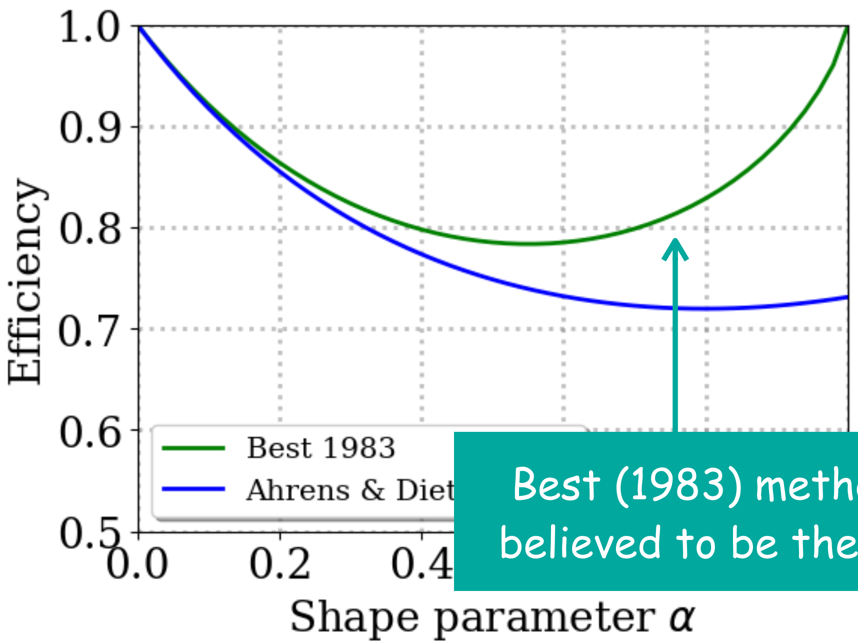
$\alpha < 1$

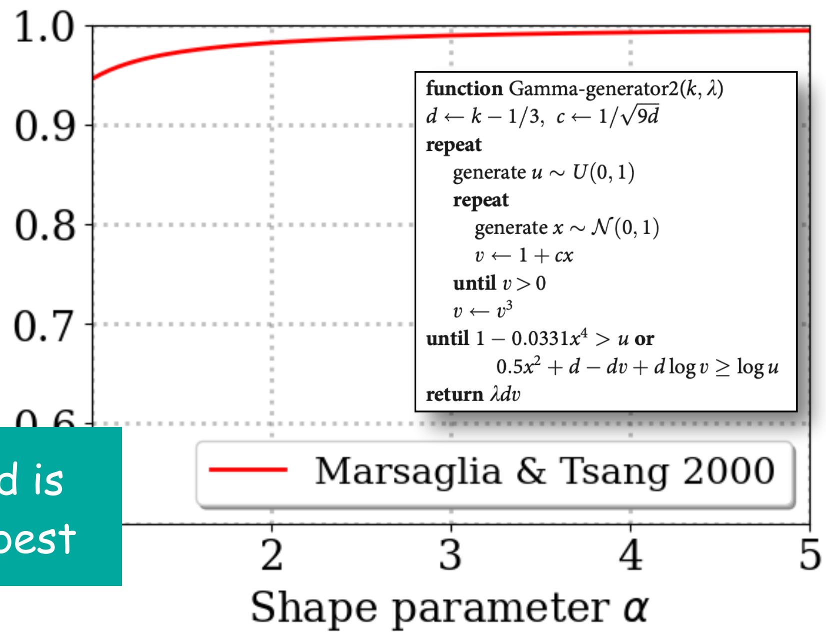
$1 < \alpha$



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



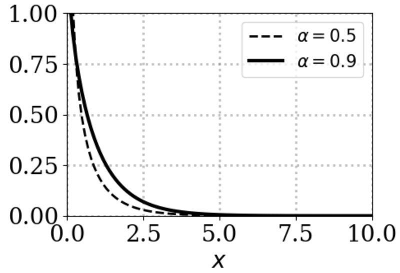




Best (1983) method is believed to be the best

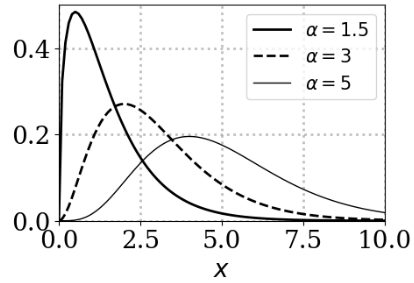
Gamma-distributed random number

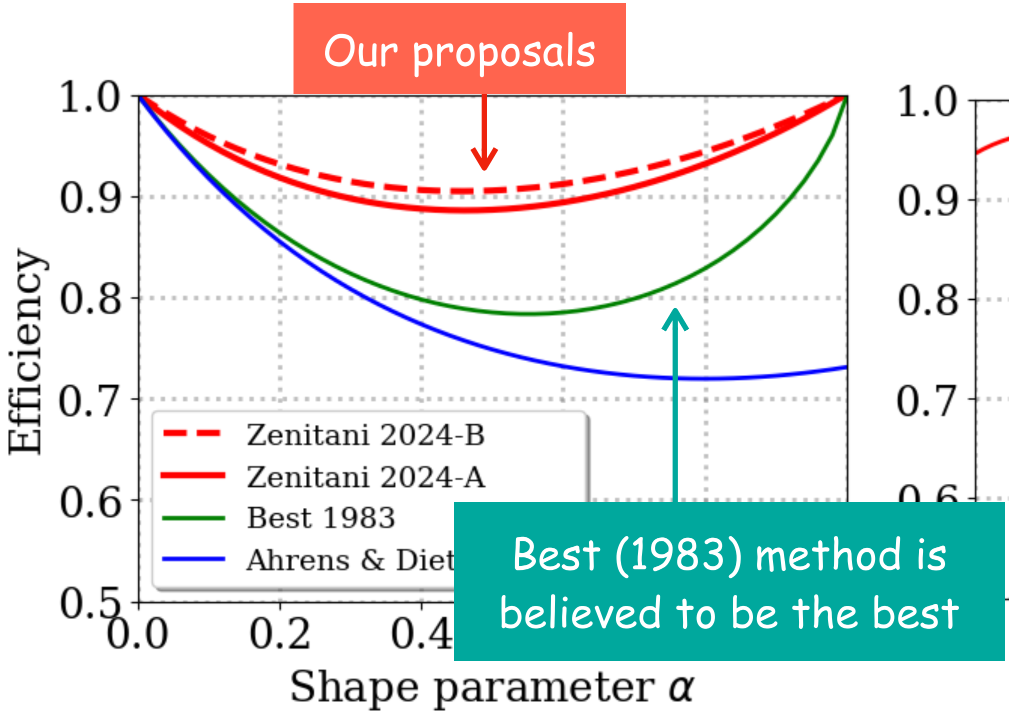
$\alpha < 1$

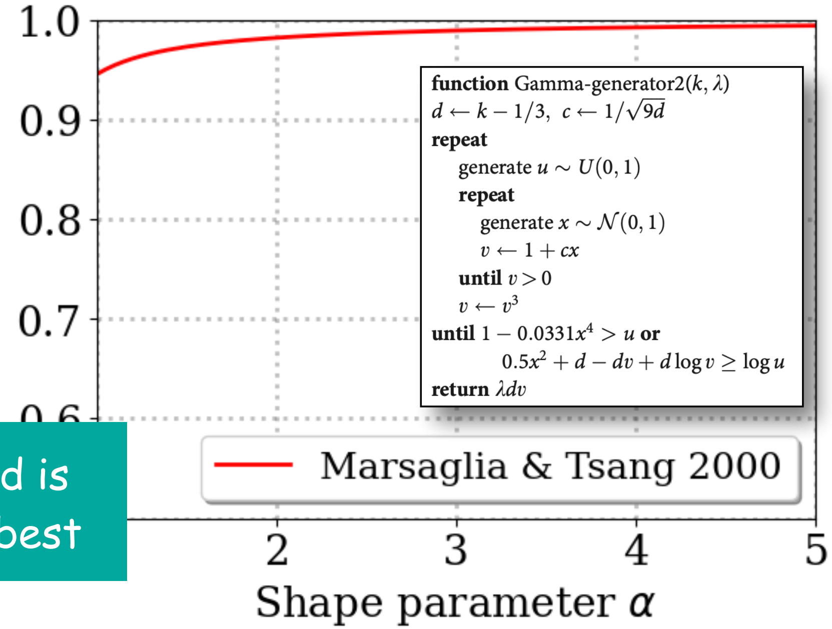


$$\mathrm{Ga}(x;\alpha,1) = \frac{x^{\alpha-1}e^{-x}}{\Gamma(\alpha)}$$

$1 < \alpha$







New gamma generator

[Zenitani 2024, Econ. Bull.]

- Generalized exponential function (Kundu & Gupta 2007)

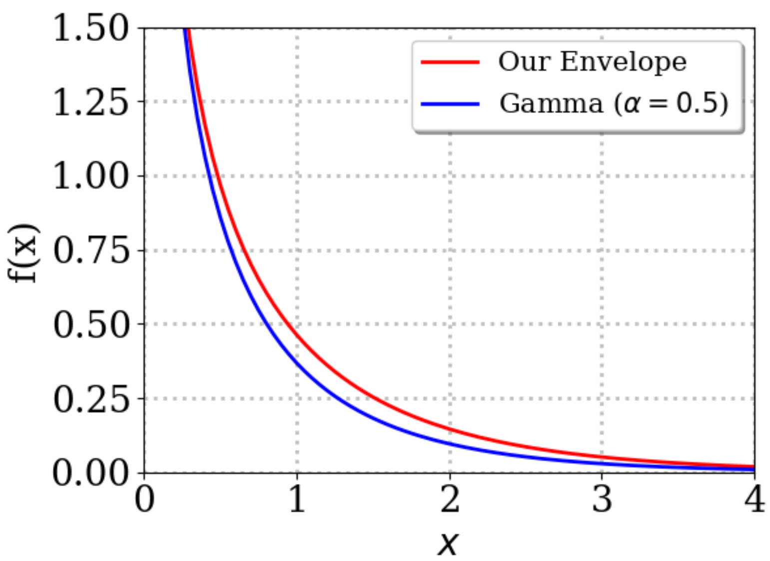
$$F_{\exp}(x;\alpha) = (1-e^{-x})^{\alpha}$$

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

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

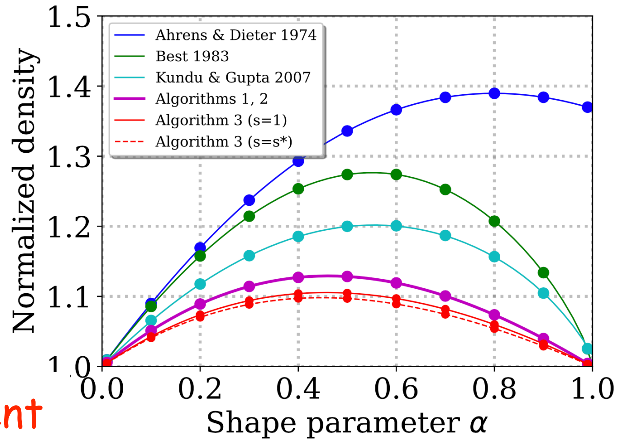
  if $U_2^{1/(1-\alpha)} x \le b$ **return** x

end repeat

New gamma generator

[Zenitani 2024, Econ. Bull.]

efficient



- A mathematical trick makes our algorithm even faster

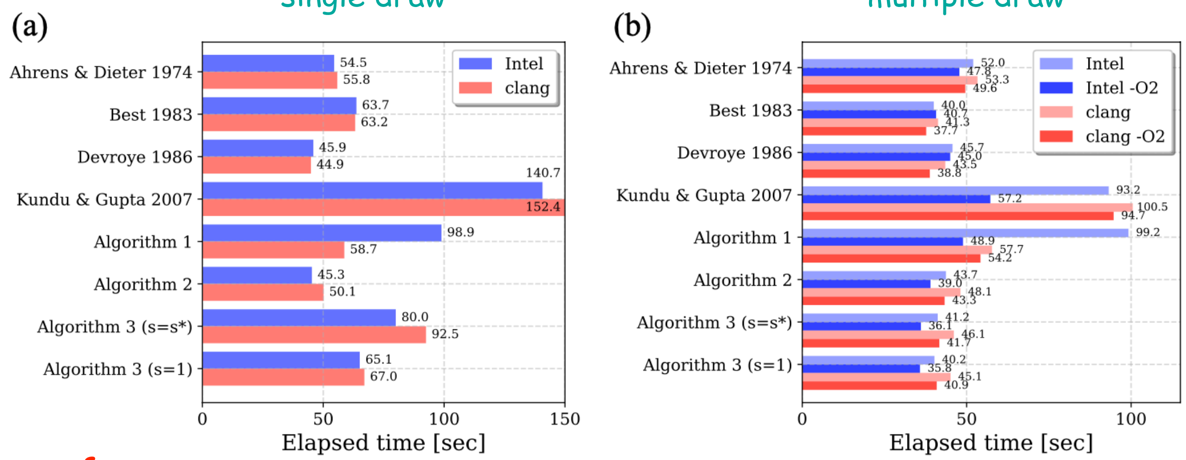
$$\frac{4+(\alpha-1)x}{4+(1-\alpha)x} \leq \left(\frac{x}{1-e^{-x}} \right)^{\alpha-1} \leq \frac{4+\alpha x}{4+(2-\alpha)x}$$

Algorithm 2

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

single draw

multiple draw



fast

Summary

These three can be combined

+

Five more

- 1. Kappa distribution
  - Normal distribution, divided by Gamma distribution
- 2. Loss-cone distribution
  - Beta distribution to scatter
- 3. Relativistic distribution
  - Superpositions of four gamma distributions
- 4. Gamma distribution
  - New generator for shape parameter less than unity

- References

  - Zenitani & Nakano, *JGR Space Physics*, 2023
  - Zenitani & Nakano, *Phys. Plasmas*, 2022
  - Zenitani, *Economics Bulletin*, 2024 (arXiv:2411.01415)

Thank you for your attention!