

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

Seiji ZENITANI

IWF, Austrian Academy of Sciences, AUSTRIA

RCUSS, Kobe University, JAPAN

Shin'ya Nakano

Institute of Statistical Mathematics, JAPAN

ÖAW

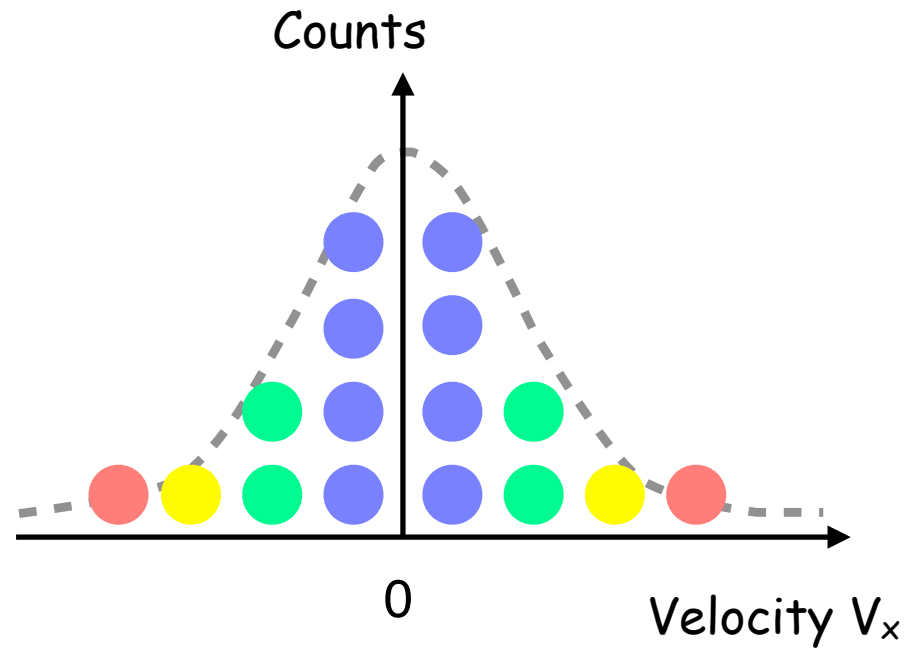
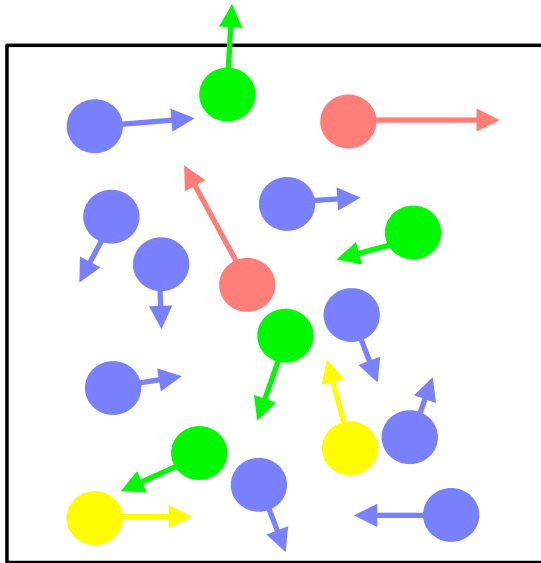
AUSTRIAN  
ACADEMY OF  
SCIENCES



KOBE UNIVERSITY

# Particle-in-cell (PIC) simulation

- It is very important to randomly prepare velocity distributions of particles in a cell



# 0. Maxwell distribution

$$f_M(\mathbf{v})d^3v = N_M \left( \frac{1}{\pi v_M^2} \right)^{\frac{3}{2}} \exp \left( -\frac{v^2}{v_M^2} \right) d^3v$$

- Normal distribution

- Box=Muller (1958) method

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

- Two random variates:  $U_1, U_2 \in (0,1)$

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

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

# 0. Maxwell distribution

$$f_M(\mathbf{v})d^3v = N_M \left( \frac{1}{\pi v_M^2} \right)^{\frac{3}{2}} \exp \left( -\frac{v^2}{v_M^2} \right) d^3v$$

- Normal distribution

- Box=Muller (1958) method

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

- Two random variates:  $U_1, U_2 \in [0,1]$

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

---

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

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

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

## Gamma distribution

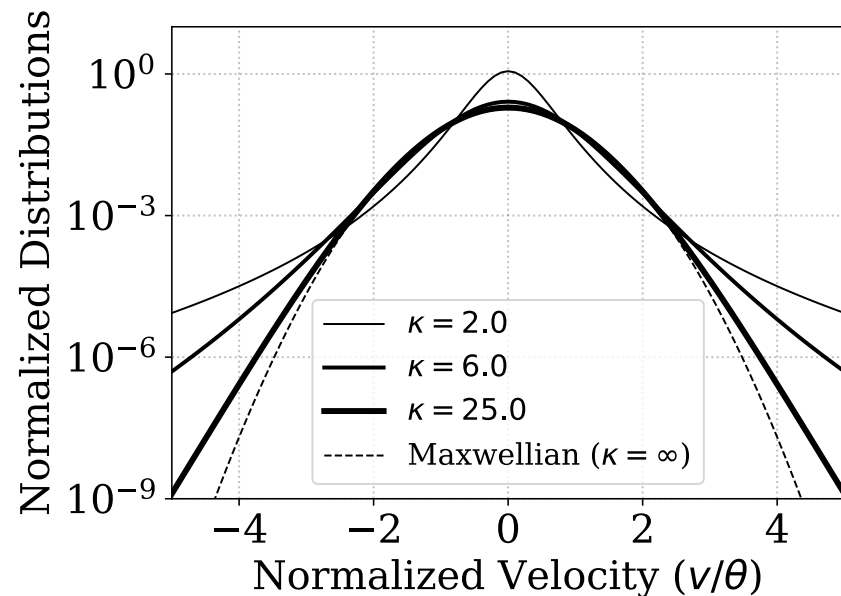
$$\text{Ga}(x; \alpha, 1) = \frac{x^{\alpha-1} e^{-x}}{\Gamma(\alpha)}$$

Gamma function

# 1. Kappa distribution

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

- Thermal core + power-law tail
- Popular in space physics  
(Vasyliunas 1968, Olbert 1968)
- $\kappa$  : power-law index
- $\kappa \rightarrow \infty$  Maxwellian



# Kappa distribution

- Spherical form  $f_{\kappa}(v)dv = N_{\kappa} \frac{4}{\pi^{1/2}(\kappa\theta^2)^{3/2}} \frac{\Gamma(\kappa+1)}{\Gamma(\kappa-1/2)} \left(1 + \frac{v^2}{\kappa\theta^2}\right)^{-(\kappa+1)} v^2 dv$   
 $= N_{\kappa} B' \left( v; \frac{3}{2}, \frac{\nu}{2}, 2, (\kappa\theta^2)^{1/2} \right) dv.$

- Generalized Beta-prime distribution

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

- Beta-prime random number

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

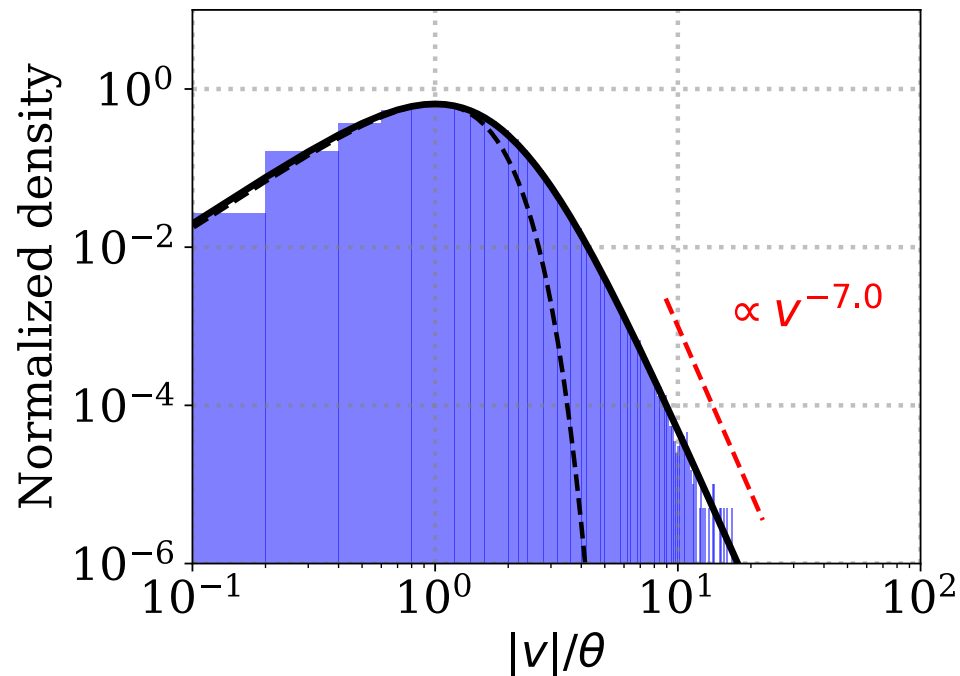
Gamma random number

Gamma random number

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

# Kappa distribution - Recipe

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



## Algorithm 1-2

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

generate  $\chi_\nu^2 \sim \text{Ga}(\kappa - 1/2, 2)$

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

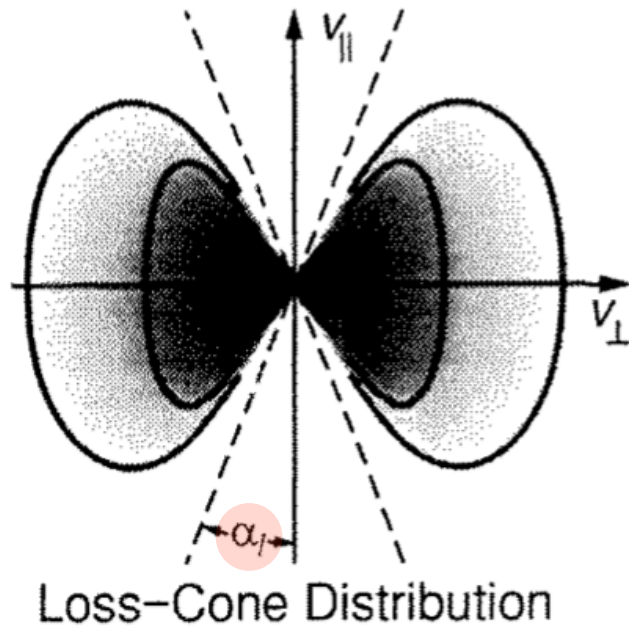
$$v_x \leftarrow rn_1$$

$$v_y \leftarrow rn_2$$

$$v_z \leftarrow rn_3$$

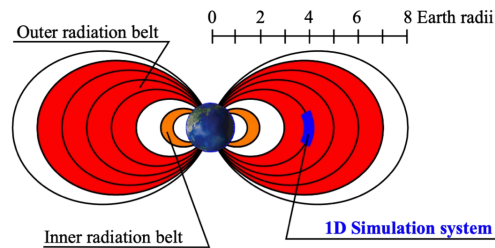
See also Abdul & Mace 2015

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



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

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

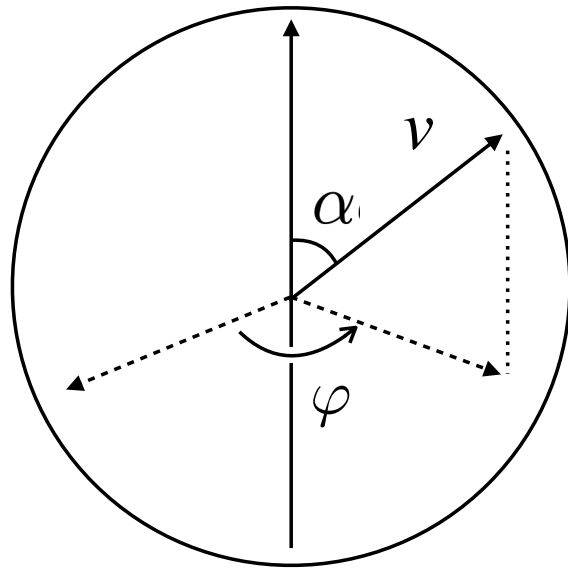


(from Katoh-san)

c.f. Kennel 1966



# Utilizing Beta distribution



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

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

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

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

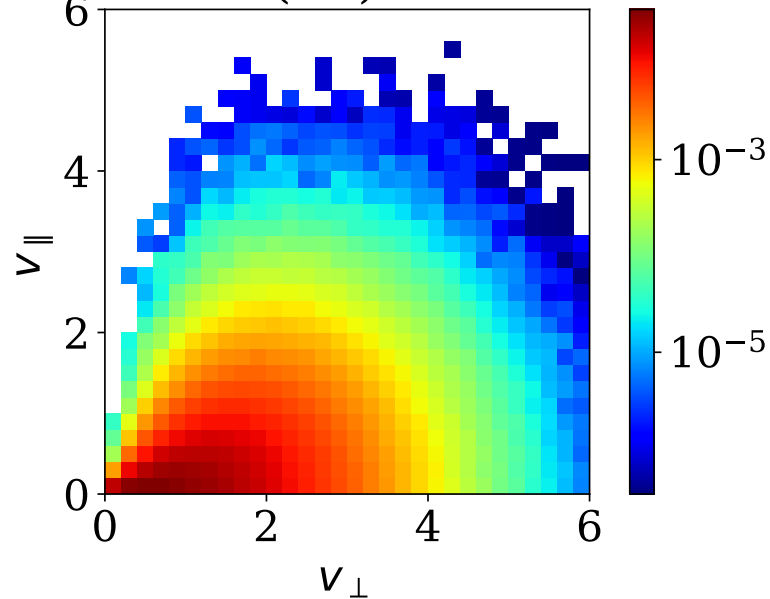
Beta function

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

Loss-cone (PA) distribution



## Algorithm 5.3: Loss-cone distribution

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

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

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

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)

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

# 3. Relativistic Maxwell distribution

(Maxwell-Jüttner distribution)

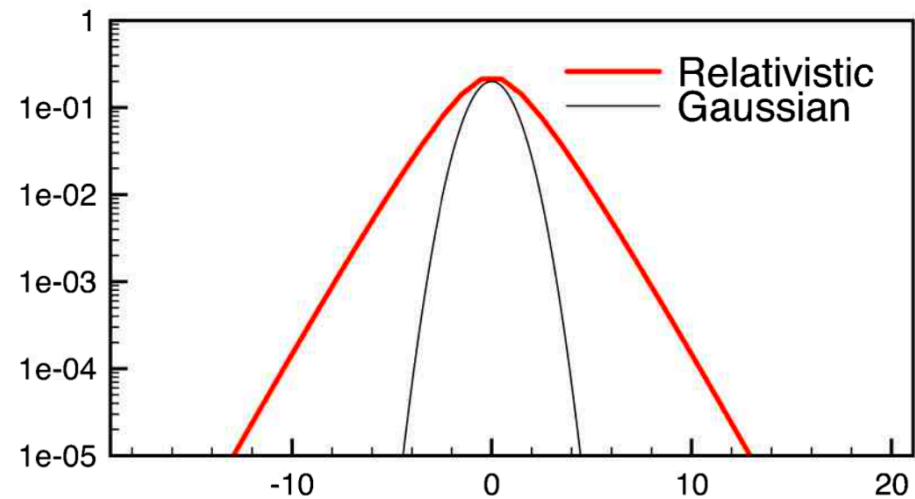
$$f_{MJ}(\mathbf{p})d^3p = \frac{N_M}{4\pi m^2 c T_M K_2(mc^2/T_M)} \exp\left(-\frac{\gamma mc^2}{T_M}\right) d^3p$$

↑  
Modified Bessel function  
of the second kind

↑  
Lorentz factor

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

- 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

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



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

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

Probability

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

Gamma distribution

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

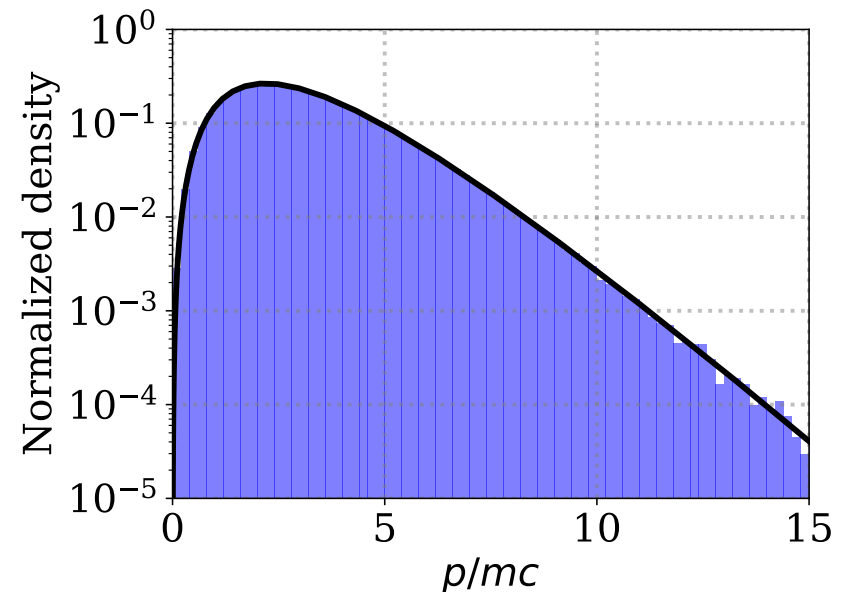
Rejection function (0.95 < R < 1.0)

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

# Modified Canfield method - Recipe

```
compute  $\pi_3, \pi_4, \pi_5$  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  $x \sim \text{Ga}(i/2, t)$  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%.



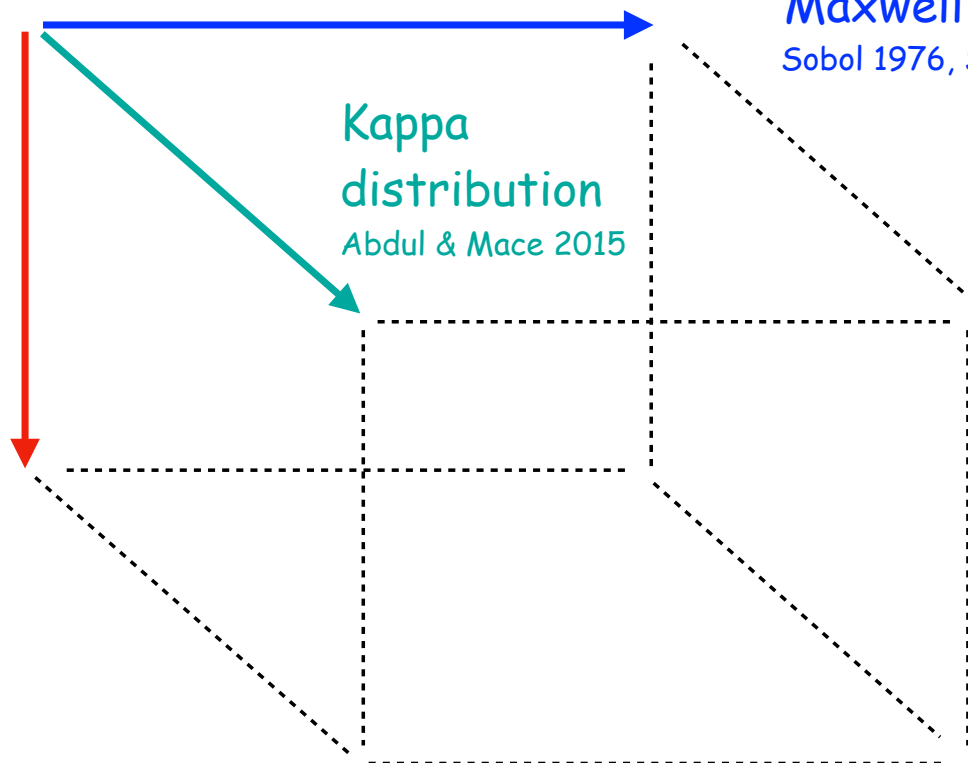
# Velocity distributions

Maxwell  
distribution  
Box=Muller 1958

Relativistic  
Maxwell distribution  
Sobol 1976, SZ & Nakano 2022

Kappa  
distribution  
Abdul & Mace 2015

Loss-cone  
distributions  
SZ & Nakano 2023



# Velocity distributions

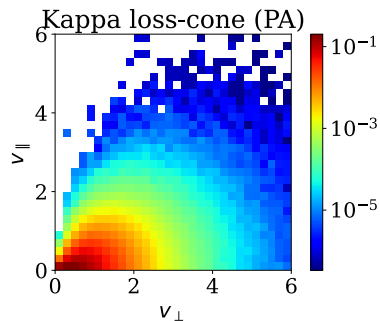
Maxwell  
distribution  
Box-Muller 1958

Relativistic  
Maxwell distribution  
Sobol 1976, SZ & Nakano 2022

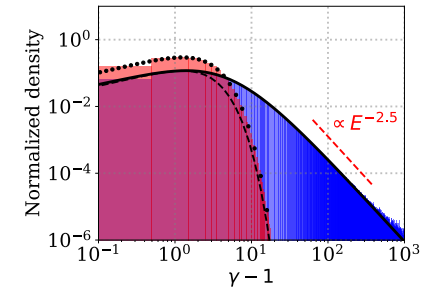
Kappa  
distribution  
Abdul & Mace 2015

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

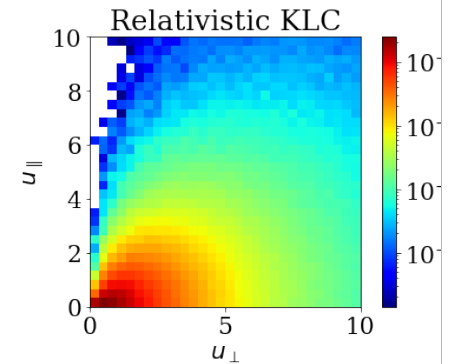
Relativistic  
kappa distribution  
SZ & Nakano 2022

Loss-cone  
distributions  
SZ & Nakano 2023

Relativistic loss-  
cone distribution

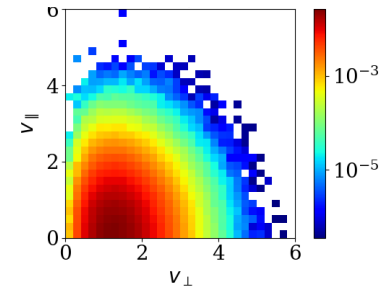
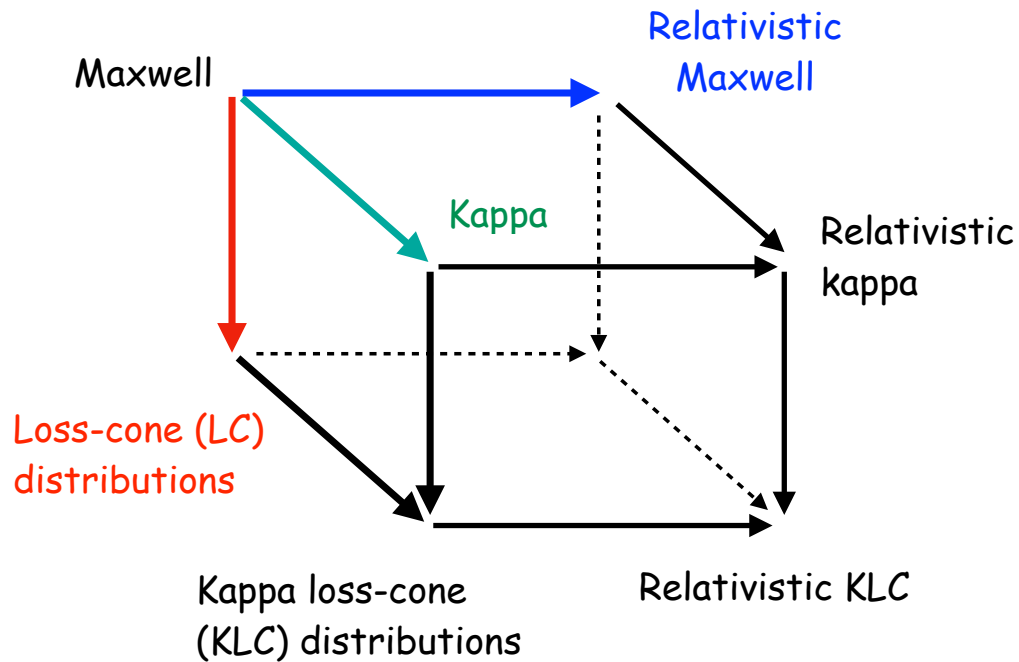
Kappa loss-cone  
(KLC) distributions

Relativistic kappa loss-cone  
(KLC) distribution



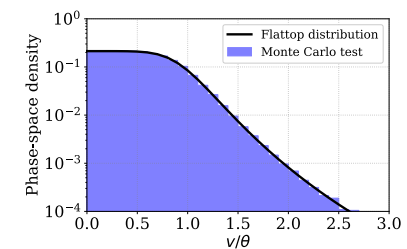


# Various distributions



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

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



# Subtracted Maxwellian

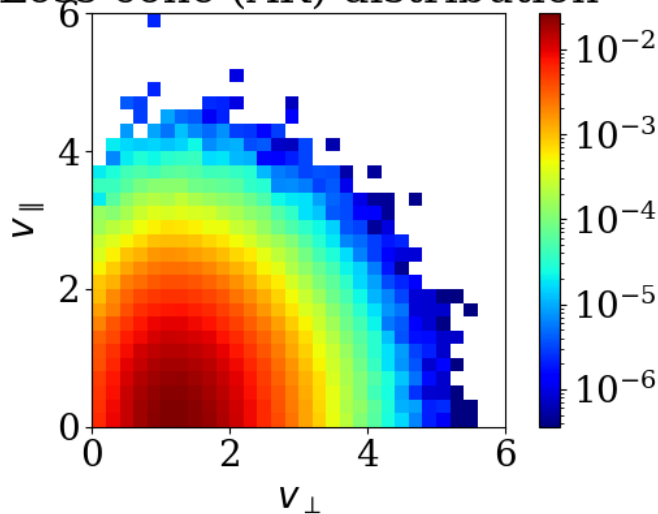
[Ashour-Abdalla & Kennel, 1978]

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

Loss-cone filling factor  $\Delta$

Shape factor  $\beta$

Loss-cone (AK) distribution



## Algorithm 2\*

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

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

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

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

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

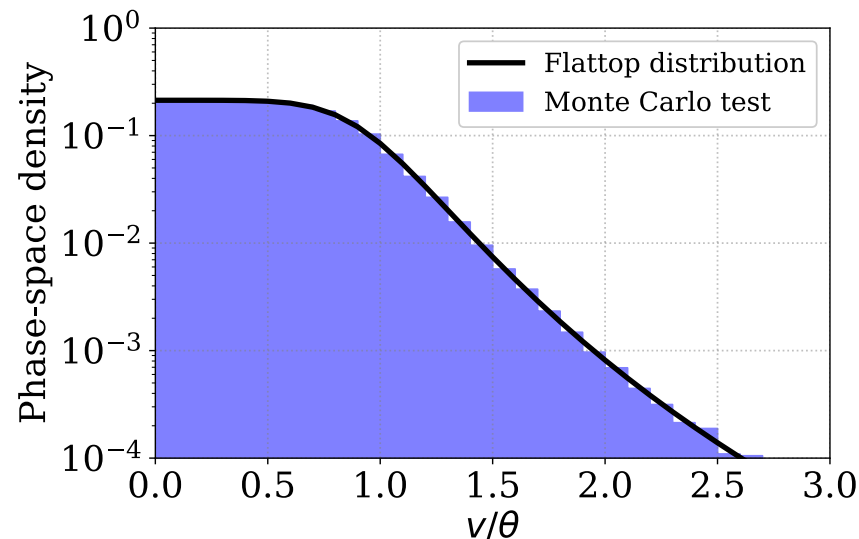
$v_{\parallel} \leftarrow \theta_{\parallel} \sqrt{1/2} N$

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

# Flattop distribution

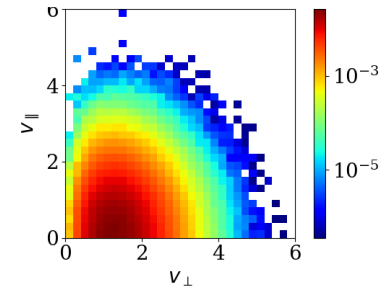
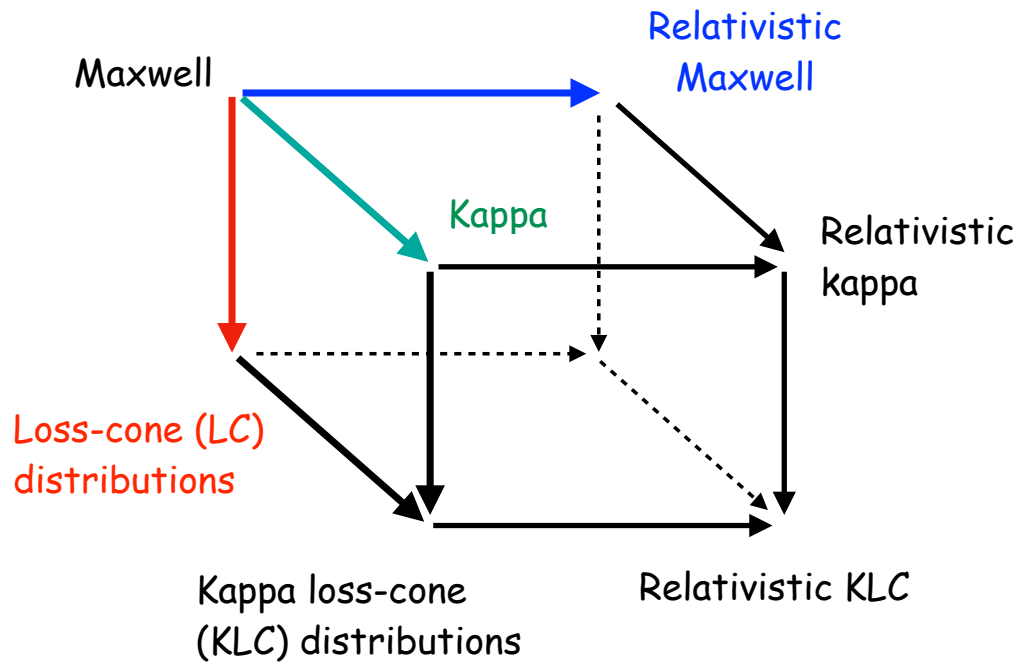
[Zenitani 2024 RNAAS]

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



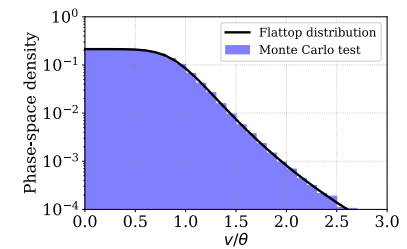
generate  $X_1 \sim \text{Gamma}(3/(2\kappa), 1)$   
generate  $X_2 \sim \text{Gamma}(1 - 1/(2\kappa), 1)$   
generate  $X_3, X_4 \sim U(0, 1)$   
 $v \leftarrow (X_1/X_2)^{1/(2\kappa)}$   
 $v_{\parallel} \leftarrow \theta_{\parallel}v (2X_3 - 1)$   
 $v_{\perp 1} \leftarrow 2\theta_{\perp}v \sqrt{X_3(1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

# Various distributions



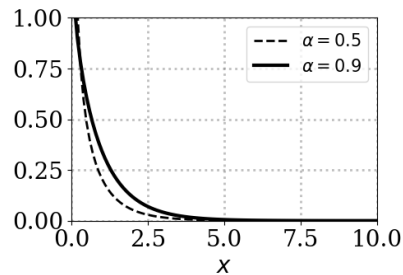
- Subtracted Maxwellian
- Dory
- Summers KLC
- Flattop
- Flattop losscone

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



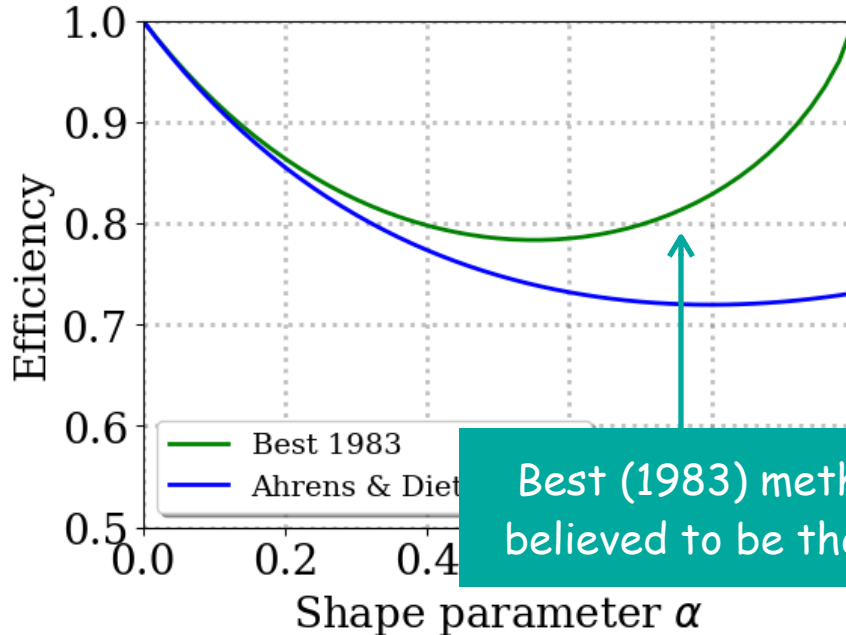
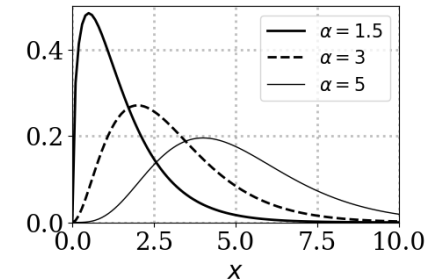
# Gamma-distributed random number

$\alpha < 1$

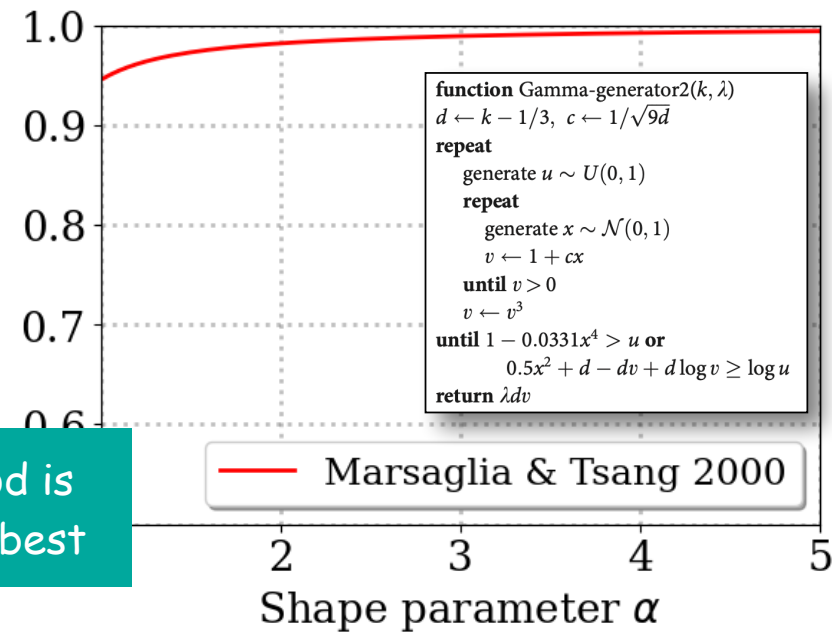


$$\text{Ga}(x; \alpha, 1) = \frac{x^{\alpha-1} e^{-x}}{\Gamma(\alpha)}$$

$1 < \alpha$



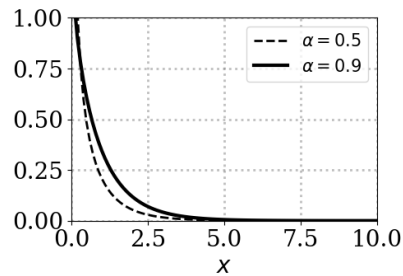
Best (1983) method is believed to be the best



```
function Gamma-generator2(k, lambda)
d ← k - 1/3, c ← 1/√(9d)
repeat
  generate u ~ U(0, 1)
  repeat
    generate x ~ N(0, 1)
    v ← 1 + cx
  until v > 0
  v ← v³
until 1 - 0.0331x⁴ > u or
      0.5x² + d - dv + d log v ≥ log u
return lambda dv
```

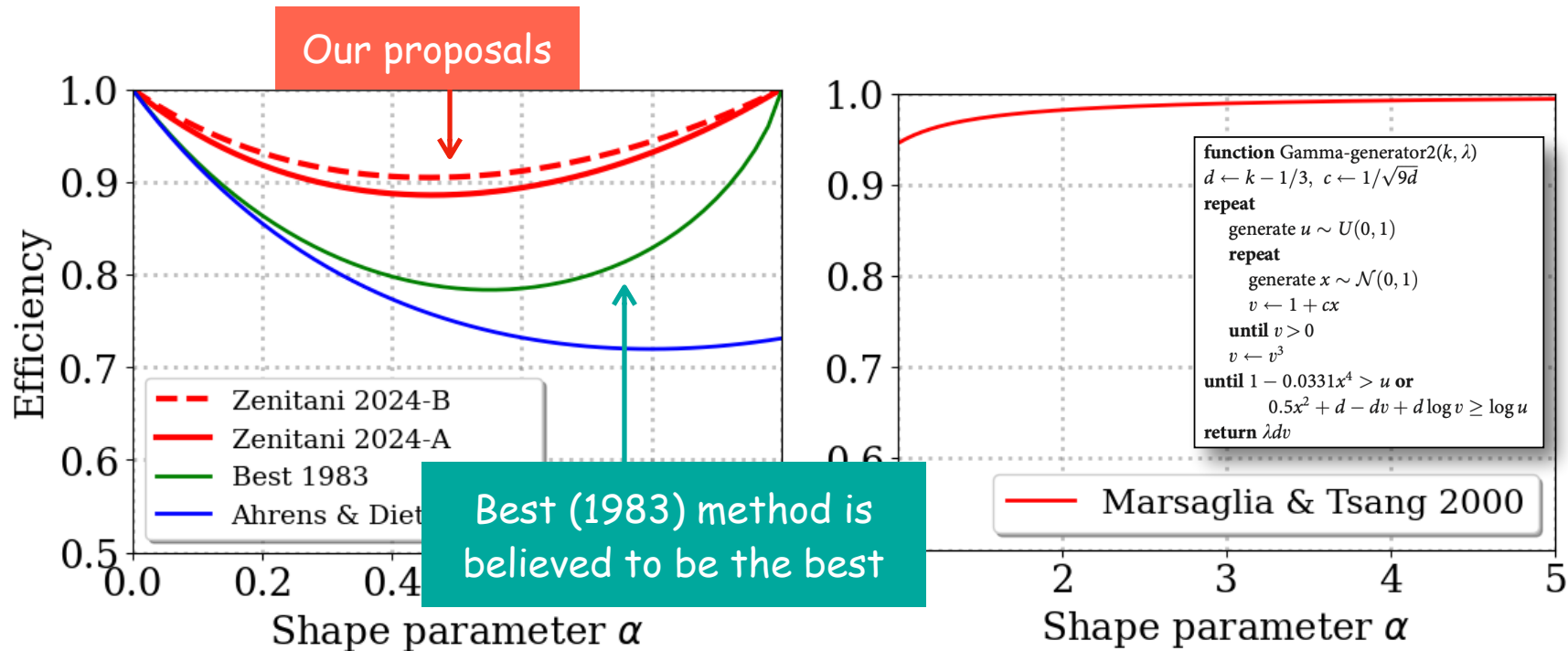
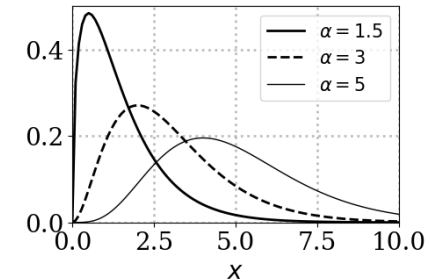
# Gamma-distributed random number

$\alpha < 1$



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

$1 < \alpha$



# New gamma generator

[Zenitani 2024, under review]

**\*\* Protected \*\***

# 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, *Phys. Plasmas*, 2022
  - Zenitani & Nakano, *JGR Space Physics*, 2023
  - Zenitani, *Economics Bulletin*, under review



Thank you for your attention!