Particle Acceleration and its numerical modeling using Monte Carlo simulations

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Outline

- Single particle motion
- Basic particle acceleration mechanisms
- Examples: Some plausible sites of particle acceleration at the Sun
- Monte Carlo simulations

Energetic particle populations in the heliosphere



Figure: Mewaldt et al. (2001)

Original figure: Kunow et al. (1991)

Single-particle motion

Equation of motion

• Charged particles obey the equation of motion

 $d\mathbf{p}/dt = q (\mathbf{E} + \mathbf{v} \times \mathbf{B}) + m\mathbf{g}$

where m, q, p and v are the particle mass, charge, momentum and velocity, and E, B and g are the electric, magnetic and gravitational field.

- Gravitational field is typically negligible, since we usually consider compact acceleration regions (mgL << W).
- dW/dt = dp/dt v = q E v, so electric fields are always required for particle acceleration. They can be either
 - potential electric fields: div **E** = ρ_q
 - induced electric fields: rot $\mathbf{E} = -\partial \mathbf{B}/\partial t$

Particle motion in slowly varying magnetic fields

 In a constant magnetic field B = B e_z, motion in the plane perpendicular to B is strictly periodic:

$$\begin{array}{l} x=r_{L}\cos{(\phi_{0}-\Omega t)} \\ y=r_{L}\sin{(\phi_{0}-\Omega t)}; \end{array} \qquad \Omega=qB/\gamma m, \ r_{L}=v/|\Omega| \end{array}$$

=> <u>Action variables</u> $J_x = \oint P_x dx$ and $J_y = \oint P_y dy$ are <u>constants</u>.

Here P = p + qA is the canonical momentum related to the Cartesian position vector r and A = -B y e_x is the vector potential of the magnetic field. Thus,

$$J_{y} = \oint \gamma m v_{y} dy = \oint \gamma m v_{y}^{2} dt = \gamma m v^{2} \pi / |\Omega| = (\pi / |q|)(p^{2} / B).$$

 If v_z ≠ 0, p should be replaced by the momentum in the plane perpendicular to the field

=>
$$p^2 \sin^2 \alpha / B$$
 = constant; cos $\alpha := \mu = v_{||} / v$

If B varies slowly, then p² sin² a/B is an <u>adiabatic invariant</u>.

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Wave-particle interactions

- Wave-particle interactions in space plasmas govern the transport of particles in rapidly fluctuating electromagnetic fields
- Consider particle motion in a monochromatic plasma wave propagating along the field line. In wave frame

 $\vec{B} = B_0 \hat{z} + B_1 [\hat{x} \cos(kz + \psi) + \hat{y} \sin(kz + \psi)]$

- Eq. of motion along the mean field \mathbf{B}_0 is $\gamma m \dot{v}_z^{(1)} = q B_1 v_\perp \sin[(k v_\parallel - \Omega)t + \psi], \quad \Omega = \frac{q B_0}{\gamma m}$
- Solution to 1^{st} order in B_1/B_0 (with $v_z = v\mu$), i.e., in quasilinear theory (QLT) is:

$$\Delta \mu = \sqrt{1 - \mu^2} \frac{qB_1}{\gamma m} \frac{\cos \psi - \cos[(kv\mu - \Omega)\Delta t + \psi]}{kv\mu - \Omega},$$

which gives $\langle \Delta \mu \rangle = 0$, when averaged over the randomly distributed phase ψ .

• Square and average over Ψ

$$\langle \Delta \mu^2 \rangle = (1 - \mu^2) \frac{q^2 B_1^2}{\gamma^2 m^2} \frac{1 - \cos[(k v \mu - \Omega) \Delta t]}{(k v \mu - \Omega)^2}$$

• Taking the limit $\Delta t \rightarrow \infty$ gives the <u>pitch-angle diffusion coefficient</u> $D_{\mu\mu} := \lim_{\Delta t \rightarrow \infty} \frac{1}{2} \frac{\langle \Delta \mu^2 \rangle}{\Delta t} = \frac{1}{2} (1 - \mu^2) \Omega^2 \frac{B_1^2}{B_0^2} \frac{\pi}{2} \delta(kv\mu - \Omega)$

 $\cos[(kv\mu]$

2 1.5

which has resonance at $k = k_r := \Omega/v\mu$!

• Take $B_1^2 = I(k)$ dk and integrate over the wavenumber spectrum

$$D_{\mu\mu} = \frac{\pi}{4} \frac{1-\mu^2}{B_0^2} \Omega^2 \int_{-\infty}^{\infty} I(k) \,\delta(kv\mu - \Omega) \,\mathrm{d}k = \frac{\pi}{4} |\Omega| (1-\mu^2) \frac{|k_r|I(k_r)|}{B_0^2}$$

- Standard QLT result: particle motion in spatially fluctuating field is diffusion in pitch-angle due to scattering off resonant plasma waves
- Taking finite wave frequencies into account, resonance condition becomes

$$\omega(k) - kv\mu = -\Omega$$

Single-particle motion: summary

 In slowly varying fields (in gyromotion scales), particles conserve their first adiabatic invariant:

 $p^2 \sin^2 a / B = constant$

- If **B** = **B**(x), also p is constant, so then (s along **B**) $(1 - \mu^2) / B$ = constant => dµ/dt = - (1- μ^2) (v/2B) ($\partial B / \partial s$) A <u>mirror force</u> directed away from strong fields!
- If **B** = **B**(t) and || z, then v_z = constant, since induced electric field is in the xy plane. Thus, choose v_z = 0 to get p^2 / B = constant (Betatron acceleration)
- In rapidly varying fields, particles interact with the fluctuations resonantly and diffuse in pitch-angle,

$$D_{\mu\mu} = (\pi/4) |\Omega| (1-\mu^2) |k_r| I(k_r) / B^2 k_r = \Omega/(v\mu);$$

where $\boldsymbol{\mu}$ and \boldsymbol{v} are measured in the frame where the fluctuation is static.

Example: focused transport equation

• As a first approximation, the interplanetary magnetic field is an Archimedean spiral:

$$B_r = B_0 (r_0/r)^2; \quad B_\phi = (\Omega_\odot r/V_{\rm sw}) B_r \propto 1/r.$$

$$B = B_r \sqrt{1 + (\Omega_{\odot} r / V_{\rm sw})^2} =: B_r / \cos \psi$$

Thus,

$$\dot{\mu} = \frac{\mu v \cos \psi}{2L} v, \ L^{1} = -\frac{\cos \psi}{B} \frac{\partial B}{\partial r}$$

 Adding the field fluctuations as pitch-angle diffusion gives the kinetic equation for solar energetic particles in the interplanetary space, i.e., the focused transport equation, as

spiral angle

$$\frac{\partial f}{\partial t} + \mu v \cos \psi \frac{\partial f}{\partial r} + \frac{1 - \mu^2}{2L} v \frac{\partial f}{\partial \mu} = \frac{\partial}{\partial \mu} \left(D_{\mu\mu} \frac{\partial f}{\partial \mu} \right); \ f = \frac{\mathrm{d}N}{\mathrm{d}\vec{x}\,\mathrm{d}\vec{p}}$$

• More complete version contains also adiabatic energy changes

Example solution (impulsive injection)







Basic particle acceleration mechanisms

DC electric fields

- "Infinitely" conducting plasma $\rightarrow E = -V \times B_{\perp} V$, B
- Particle acceleration by DC electric field requires either
 - $\mathbf{E} \cdot \mathbf{B} \neq 0$ (resistive plasma),
 - $\mathbf{B} \approx 0$ (magnetic null point / line), or
 - Strong curvature / gradient drifts across the magnetic field
- Available, e.g., in reconnection regions





static current sheet, **E** = 0

reconnecting current sheet, $\mathbf{E} \neq \mathbf{0}$

- Particle motion relatively straightforward to compute
- Challenges in the self-consistent description of the E-field
 - reconnection in collisionless plasmas (no classical resistivity)
 - 3-D reconnection fields

Shock-drift acceleration (Hudson 1965)

- operates in MHD shocks (discontinuities)
- particles energized by the convective DC electric field
- net gradient + curvature drift along the E-field for ions and against the E-field for electrons
- single interaction provides only a small energy gain, $W_2 \sim (B_2/B_1) \cdot W_1$
- in oblique shocks, largest energy gains for reflected ions



Shock drift acceleration in inhomogeneous magnetic fields

- Single encounter with an MHD shock does not yield large energies
- Shock drift acceleration in inhomogeneous upstream magnetic field
 - inhomogeneous upstream fields can trap particles close to the shock resulting in multiple interactions with the shock
 - trapped particles gain energy if
 - dB₁ / dt > 0 (W/B₁ = const.), or
 - $\Theta_{\rm n} \rightarrow 90^{\rm o}$ (v_{||} ~ V_s/cos $\Theta_{\rm n} \rightarrow$ c)
 - both possible in coronal shocks



Sandroos & Vainio (2006: A&A 455, 685)

Acceleration in curved upstream field



Fig. 2. Setup for line current runs. At t = 0 the shock plane is situated 10 keV protons are injected to the field line marked with a diamond. Magnitude of B is shown with the contour lines, along with two field lines.

Fig. 3. Initial pitch angle vs. energy gain ratio $\Delta E/E_0$ for a line current at x = 0 (dashed line) and moves from right to left with velocity V_s . run with $V_s = 400 \text{ km s}^{-1}$ and r = 4. Each dot is one simulated particle.

Sandroos & Vainio (2006: A&A 455, 685)

Shock surfing acceleration (Sagdeev 1966)

 Kinetic collisionless shock: charge separation caused by ion inertia leads to a cross-shock potential field

 $E_x = -d\phi/dx$,

which points towards the upstream region

• E_x-field estimated by

 $e \delta \phi < \frac{1}{2}m_i V^2, \delta x > c/w_{pe}$

 Part of the incoming ions get reflected by E_x repeatedly and, thus, accelerated in -y direction along the convective E_y field until

$$-e v_y B_z \sim e E_x$$

MeV energies in coronal shocks?



Stochastic acceleration

- Wave-particle interactions with EM plasma waves
 - Cyclotron resonance condition $\mathbf{w} = \mathbf{v}_{||} \mathbf{k} + \mathbf{n} \boldsymbol{\Omega}$ where $\mathbf{n} \in \mathbb{Z}$



Example: Stochastic acceleration and impulsive flares



Petrosian & Liu (2004: ApJ 610, 550) Liu & al. (2004: ApJ 613, L81) Liu & al. (2006: ApJ 636, 462)

- Puzzle: impulsive solar flares seem to produce a huge overabundance of accelerated 3-He over alphas
- Thermal protons and alphas damp resonant waves → acceleration of protons and alphas requires supra-thermal energies
- 3-He and heavies not abundant enough to damp resonant waves → effective injection into the acceleration process
 - So far applied to impulsive flares:
 - Explains abundance enhancements of 3-He in impulsive flares
 - Very sensitive to f_{pe}/f_{ce}



Liu & al. (2006: ApJ 636, 462)

Diffusive shock acceleration





Particles crossing the shock many times (because of strong scattering) get accelerated

DSA Spectrum (e.g., Bell 1978)

The mean momentum after n shock crossings

 $\langle p_n \rangle = p_0 \exp(\frac{4}{3} \sum_{j=1}^n \Delta u / v_j)$

Probability of returning to the shock after n crossings

$$P_n = \exp(-4\sum_{j=1}^n u_2/v_j)$$



Geometry of diffusive shock acceleration

 DSA spectral index does not depend on geometry, but the rate of DSA does (Drury 1983)

 $dp/dt = p [(r_{sc}-1)/3r_{sc}] \cdot (u_{1x}^{2} / D_{xx})$ $D_{xx} = Dcos^{2}\theta_{n}; \quad D = \Lambda v/3$

- Time available $t_{acc} = (\Delta s/u_{1x}) \cos \theta_n$
- For a given Λ

 $v_{max} \sim (\Delta s / \Lambda) \cdot (u_{1x} / \cos \theta_n)$

But: Injection of protons requires

 $v_{inj} \sim u_{1x} / \cos \theta_n$

- Thus, quasi-perpendicular shocks
 - require higher injection energies but
 - accelerate particles to higher energies than quasi-parallel shocks



Vainio (2006)

Selection effect of shock geometry



Plausible sites of particle acceleration in solar plasmas

Bow shocks and refracting shocks



Reconnecting current sheets and turbulent sheath regions



FIG. 1.—Evolution of plasmoid eruption. The contour lines represent magnetic field lines, the black arrows represent the fluid velocity field, and the color map represents temperature. The yellow arrows show the positions of the piston-driven fast shock and the reverse fast shock.

Magara et al. (2000: ApJ 538, L175)



Figure 3. The cartoon shows the resonant acceleration sites of (A) electrons and most ions and (B) ³He by electron-generated EMIC waves. Particles escape to 1 AU at the top of the figure, produce neutrons, X- and γ -rays in the loop footpoints, and electrons emit radio bursts along the legs of the loop.

Reames (2000)

Test-particle modeling of particle acceleration using the Monte Carlo method

Test-particle-orbit simulations

- Probably the simplest way to study the evolution of accelerated particle populations is to perform test-particle-orbit simulations
 - Take the EM fields as prescribed fields of **r** and t
 - Trace a population of charged particles (using a standard Lorentzforce solver) in the fields keeping track of their position and momentum as a function of time
 - Collect the statistics at some intervals of time and study how the particle distribution evolves
- Problem: Any acceleration model that involves resonant wave-particle interactions needs to resolve the fluctuating fields at sub-Larmor scales
 - Strongly limits the use of test-particle-orbit simulations in cases, where the acceleration region is spatially extended (L >>> r_L) or the acceleration process is slow (T >>> Ω^{-1})
 - DSA is a prime example of such a mechanism

Monte Carlo simulations

- If the size of the system is large, it is not possible to keep track of Larmor motion -> use guiding-center theory to propagate particles in the large-scale fields
- How to implement the effect of small-scale fluctuations? Use quasilinear theory to account for the effects of turbulent fluctuations, I(k)
- Thus, particle motion is modeled as a combination of deterministic motion in large scale fields and stochastic motion (scattering) in small scale fields
- Advantage: solver is no longer limited by time steps $\Delta t \ll \Omega^{-1}$ since gyromotion is not followed at all
- Limitation: the treatment is (formally) limited to weak turbulence:

 $\delta B^2 \sim k I(k) \ll B^2$ at all $k > \Omega/v$

• However, qualitatively correct results can be obtained even for

Example: particle motion in magnetostatic slab-mode turbulence

- Consider a system with a homogeneous mean magnetic field $\mathbf{B}_0 = \mathbf{B}_0 \mathbf{e}_z$ and a turbulent field $\mathbf{B}_1 = \mathbf{B}_{1x}(z) \mathbf{e}_x + \mathbf{B}_{1y}(z) \mathbf{e}_y$ with $\mathbf{B}_1 \leftrightarrow \mathbf{B}_0$.
- Let the statistics of the turbulent field be same in both x and y and be represented by a power spectrum

 $I(k) = I_0 (k/k_0)^{-q}, k > k_0$

• Particle motion in the regular field is simply described by

$$dz/dt = v\mu \rightarrow \Delta z = v\mu \Delta t$$

 Particle motion in the turbulent field is diffusion in µ. It can be modeled in several ways. In general, a distribution under pitch-angle diffusion evolves according to

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial \mu} \left(D_{\mu\mu} \frac{\partial f}{\partial \mu} \right) = \frac{1}{2} \frac{\partial^2}{\partial \mu^2} (2D_{\mu\mu}f) - \frac{\partial}{\partial \mu} \left(\frac{\partial D_{\mu\mu}}{\partial \mu}f \right)$$
$$D_{\mu\mu} = \frac{\pi}{4} |\Omega| (1-\mu^2) \frac{|k_r|I(k_r)}{B^2}; \qquad k_r = \frac{\Omega}{v\mu}$$

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial \mu} \left(D_{\mu\mu} \frac{\partial f}{\partial \mu} \right) = \frac{1}{2} \frac{\partial^2}{\partial \mu^2} (2D_{\mu\mu} f) - \frac{\partial}{\partial \mu} \left(\frac{\partial D_{\mu\mu}}{\partial \mu} f \right)$$

• Thus, the diffusion equation is equivalent to the Fokker-Planck equation:

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial \mu} \left(\frac{\langle \Delta \mu \rangle}{\Delta t} f \right) + \frac{1}{2} \frac{\partial^2}{\partial \mu^2} \left(\frac{\langle \Delta \mu^2 \rangle}{\Delta t} f \right)$$

• We can now identify the mean displacement and mean square displacement as $\langle \Delta \mu \rangle = \partial D_{\mu\mu} = \langle \Delta \mu^2 \rangle$

$$\frac{\langle \Delta \mu \rangle}{\Delta t} = \frac{\partial D_{\mu\mu}}{\partial \mu}; \quad \frac{\langle \Delta \mu^2 \rangle}{\Delta t} = 2D_{\mu\mu}$$

• If the time steps are small enough (to keep changes in μ small), we can thus write

$$\Delta \mu = \frac{\partial D_{\mu\mu}}{\partial \mu} \Delta t + W \sqrt{2D_{\mu\mu}\Delta t}$$

where W is a normally distributed random number. This allows one to construct a 1st order Euler solver for the stochastic particle motion.

$$z_{n+1} = z_n + v\mu_n \Delta t$$

$$\mu_{n+1} = \mu_n + \frac{\partial D_{\mu\mu}}{\partial \mu} (z_n, \mu_n) \Delta t + W \sqrt{2D_{\mu\mu}(z_n, \mu_n) \Delta t}$$

Generating "random" numbers on a computer

- As all stochastic simulations need some sort of random numbers, let us take a brief look at issues that need to be understood
- Firstly, one needs a good random number generator that produces (pseudo) random numbers between 0 and 1
- Never use random generators that you do not have documentation for. Many of them are simply flawed.
- The simplest generators are linear congruental generators (LGC):

 $X_{n+1} = (a X_n + c) \mod m$, $R_n = X_n / m$

where a, c and m are (integer) parameters. Choosing the parameters badly will lead to poor results.

- One of the "recommendable" LCGs is the Park-Miller "Minimal Standard" (PMMS) generator obtained with a=16807, m=2³¹-1, c=0. Its properties are well known and it passes the most obvious statistical tests quite well.
- It is recommendable to test the code using a few different types of generators (PMMS, ran2, Mersenne twister). If the results agree, the one with the lowest running time is probably fine.

Sampling from different distributions

- Assuming that you have a good pseudo-random number generator at hand, you often still need to draw numbers from other than uniform distribution.
- Example: Generating random numbers distributed exponentially in $[0,\infty)$.
 - Let y be a random variable with a probability density

f(y) = exp(-y)

Let F be a function of y and ass. dF = f(y) dy with F(0)=0.
 Thus, F is a uniformly distributed variable in [0,1) and

 $F(y) = \int_{0}^{y} f(y) dy = 1 - exp(-y) \implies y = -\ln(1-F)$

Thus, F ~ Uni[0,1) => X = 1-F ~ Uni(0,1] => y = -ln X ~ Exp(μ=1).

Generating normally distributed numbers (two at a time) can be done easily as well. Using polar coordinates x=r cosθ; y=r sinθ, we get f(y,x) dxdy ~ exp{-½(x²+ y²)} dxdy = exp{-½r²} rdr dθ = ½exp{-½r²} d(r²)dθ r² ~ Exp(μ=2) and θ ~ Uni(0,2π) => x, y ~ N(μ=0,σ=1).

Efficiency issues

- Although simple, the 1st order Euler solver is not very efficient in terms of computational time, since the method works accurately only if the displacements in μ are very small. This is rather limiting, since $\Delta \mu \sim \int \Delta t$.
- In special cases for $D_{\mu\mu}$, much more efficient solvers can be constructed from more accurate solutions of the pitch-angle diffusion equation.
- In the case of isotropic angular diffusion,

$$\mathsf{D}_{\mu\mu}\sim 1-\mu^2,$$

the solution of the angular distribution can be given analytically.

• The equivalent solution for μ after each scattering is

$$\mu_{n+1} = \mu_n \cos \theta + \sqrt{1 - \mu_n^2} \sin \theta \cos \varphi$$

$$\theta^2 = -\frac{4D_{\mu\mu}\Delta t}{1 - \mu^2} \ln R_{2n}; \quad \varphi = 2\pi R_{2n+1}$$

where R_n is a sequence of random numbers distributed uniformly in (0,1]. The angles Θ and φ are the scattering angles relative to the propagation direction prior to scattering



Particle propagator under isotropic pitchangle diffusion

Ass. $D_{\mu\mu} = (1 - \mu^2)\nu$

We now have a recipe to solve the stochastic motion of N particles in the fluctuating field from t = 0 to t = T:

- 1. Choose the time step $\Delta t = T/K$, where K is a large enough integer so that $4\nu\Delta t \ll 1$ and put the particle counter i = 0.
- 2. Inject a new particle at $z = z_0$, $v = v_0$ and $\mu = \mu_0$, and update the particle counter $i \leftarrow i + 1$.
- 3. Move the particle in the z-direction using $z \leftarrow z + v\mu\Delta t$
- 4. Scatter the particle:
 - (a) pick random numbers $\theta^2 = -4\nu\Delta t \ln R_1$ and $\varphi = 2\pi R_2$, where $R_1 \in (0, 1]$ and $R_2 \in (0, 1]$ are random numbers picked from uniform distribution. θ and φ are the scattering angles relative to the present particle propagation direction.
 - (b) Use spherical trigonometry to calculate the new pitch-cosine

$$\mu \leftarrow \mu \cos \theta + \sqrt{1 - \mu^2} \sin \theta \cos \varphi$$

- 5. Update the time $t \leftarrow t + \Delta t$
- 6. If t < T, go to 3
- 7. If i < N, go to 2
- 8. End

Particle acceleration - regular E

- So far, we considered a very simple model with v = const. (No E field.)
- Depending on the acceleration mechanism, the best implementation of particle acceleration to a MC simulation varies.
- For E perpendicular to B₀ (and not too large), it is possible to make a coordinate transformation to a frame, where E vanishes (at least locally) and consider the propagation step there. Note that in general the frame is not an inertial frame.
- Consider then a large-scale E || B₀. Thus, the regular motion between magnetic scatterings can be integrated exactly (for E = const): Just replace step 3 above by

$$w_{n} = v_{n}\mu_{n}$$

$$w_{n+1} = w_{n} + (q/m)E\Delta t$$

$$z_{n+1} = z_{n} + \frac{1}{2}(w_{n} + w_{n+1})\Delta t$$

$$v_{n+1} = \sqrt{w_{n+1}^{2} + v_{n}^{2} - w_{n}^{2}}$$

$$\mu_{n+1} = w_{n+1}/v_{n+1}$$

• After the regular motion, magnetic scattering can be performed as above.

Particle acceleration – fluctuating E

- Effects of turbulent E are more complicated to implement and, again, the best choice of a method depends on the particular case.
- We will, as a first approximation, consider only electric fields that are due to MHD-wave and fluid-scale turbulent processes. The turbulent electric field in the rest frame of the background plasma ($V_0 = 0$) is typically

 $E_1 \sim V_1 B_0 \sim V_A (B_1/B_0) B_0 = V_A B_1$,

where V_1 is the (turbulent) plasma velocity fluctuation.

- Note that V_A << v, if energetic particles are considered, so v B₁ >> E₁! Thus, as the lowest order approximation, scattering can be considered elastic (v = const.) in the local background plasma frame.
- Thus, to implement the effect of such fields, all one has to do is to
 - transform to the local plasma frame before each scattering
 - perform the scattering as in magnetostatic turbulence
 - transform back to the laboratory frame.

This implements, e.g., the 1st order Fermi mechanism at shocks.

Stochastic acceleration

- Stochastic acceleration occurs, because the particle is able to scatter off waves propagating at different phase velocities simultaneously.
- To implement this effect one has to consider scattering off at least two wave fields (e.g., with $\omega = {}^{\pm} V_A k$) after each propagation step.
- In the frame co-moving with the wave, the field is again static (no E-field). Thus, in the wave frame scattering is elastic.
- Thus, after each propagation step,
 - transform to the local wave frame before each scattering (at least two scatterings after each propagation step)
 - perform scatterings as in magnetostatic turbulence
 - transform back to the laboratory frame.

This implements the stochastic acceleration mechanism