DKE Solver NEO-2: Field Line Tracing Revisited*

Winfried Kernbichler[1], Sergei V. Kasilov[2], Georg Leitold[1]

[1]Institut für Theoretische Physik
Technische Universität Graz
Petersgasse 16, A–8010 Graz, Austria

[2]Institute of Plasma Physics
National Science Center "Kharkov Institute of Physics and Technology"
Ul. Akademicheskaya 1, 61108 Kharkov, Ukraine

*Association EURATOM-ÖAW

Kinetic Theory in Stellarators, Graz, September 13 - 15, 2004

Problems with Existing Solvers

- **DKES and conventional MC**
  best suited for collisional regimes
  all regions of phase space treated in the same manner
  slow convergence, long run-times in low collisional regime
  no integral part of the linearized collision operator

- **GSRAKE**
  limited to multiple-helicity model

- **NEO**
  low collisionality, no E_r, only pitch angle scattering

- **SMT** (high dimensional problems, convection, ECRH)
  assumption of low collisionality violated in the region around trapped-passing boundary

Open Physics (and not Physics) Problems

- Bootstrap current in low collisionality regimes
  effect mainly determined by region around trapped-passing boundary
  proper treatment of collisions for these particles is crucial
- Calculation of current drive efficiencies
  generalized Spitzer functions are the main tool for ECRH, NBI and other methods
  2D in tokamaks - 4D in stellarators
  simplification of collision integrals leads to problems
- Fast solver for balance problems
  or for filling the database
- Degradation of the performance of most DKE solvers in LMFP regime - steep behaviour of f across t-p boundary and boundaries between t-classes
  how to create an adaptive grid in phase space
- Solver for general equilibria
  PIES, HINT (or just from coil currents)
  how to avoid magnetic coordinates in a general solver
- SMT needs propagators for the phase space regions where collisions cannot be considered by a perturbation theory in the LMFP regime (near t-p boundary)

Questions - And a Vision

- Can one build on the strength of field line tracing
  - good convergence in the low collisionality regime
  - no immediate need for magnetic coordinates
  - relatively easy (e.g., compared to SMT)
  - fast
- and construct a general solver?
  - which works in all collisionality regimes
  - which includes drive from inductive parallel electric fields
  - which effectively resolves steep behaviour of f
  - which uses the full linearized collision operator
  - which allows for radial electric fields
- Let's start with all collisionality regimes (and parallel electric fields)
- and look ahead to the full collision operator and to $E_r \neq 0$

Drift Kinetic Equation

$$\sigma \frac{\partial \tilde{f}^\sigma}{\partial s} - \frac{\partial}{\partial J_\perp}\left(4\nu \frac{|v_\parallel| J_\perp}{B}\frac{\partial \tilde{f}^\sigma}{\partial J_\perp}\right) = \frac{\partial}{\partial J_\perp}\left(\frac{|v_\parallel|}{B} V_G \frac{\partial f_M}{\partial \psi}\right)$$

with normalization and

$\hat{V}_G = \frac{1}{3}\left(\frac{4}{\hat{B}} - \eta\right)|\nabla\psi| k_G$	radial drift velocity
$|\nabla\psi| k_G$	geodesic curvature
σ	sign of $v_\parallel$
$\eta = (1-\lambda^2)/\hat{B}$	dimensionless perpendicular action
$\tilde{f}^\sigma = \frac{v}{\omega_{c0}} \frac{\partial f_M}{\partial \psi} \hat{f}^\sigma$	distribution function

turns into

$$\sigma \frac{\partial \hat{f}^\sigma}{\partial s} - \kappa \frac{\partial}{\partial \eta}\left(\frac{|\lambda| \eta}{\hat{B}}\frac{\partial \hat{f}^\sigma}{\partial \eta}\right) = \frac{\partial}{\partial \eta}\left(\frac{|\lambda|}{\hat{B}} \hat{V}_G\right)$$

Particle Flux Density

Averages over flux surfaces expressed through field line integrals

$$F_n = -\pi \lim_{L\to\infty} \left(\int_0^L \frac{\mathrm{d}s}{B} |\nabla\psi| \right)^{-1} \sum_{\sigma=\pm 1} \int_0^L \mathrm{d}s \int_0^\infty \mathrm{d}v\, v \int_0^{v^2/B} \mathrm{d}J_\perp \tilde{f}^\sigma \frac{\partial}{\partial J_\perp} \frac{|v_\parallel|}{B} V_G$$

$$= \pi \int_0^\infty \mathrm{d}v \frac{v^5}{\omega_{c0}^2} \frac{\partial f_M}{\partial \psi} \lim_{L\to\infty} \left(\int_0^L \frac{\mathrm{d}s}{B} |\nabla\psi| \right)^{-1} \sum_{\sigma=\pm 1} S^\sigma(L)$$

$$\frac{\mathrm{d}S^\sigma(s)}{\mathrm{d}s} = -\int_0^{1/\hat{B}} \mathrm{d}\eta \hat{f}^\sigma \frac{\partial}{\partial \eta} \frac{|\lambda|}{\hat{B}} \hat{V}_G = \int_0^1 \mathrm{d}|\lambda| \hat{f}^\sigma \frac{\partial}{\partial |\lambda|} \frac{|\lambda|}{\hat{B}} \hat{V}_G$$

$$S^\sigma(0) = 0$$

Parallel Current Density

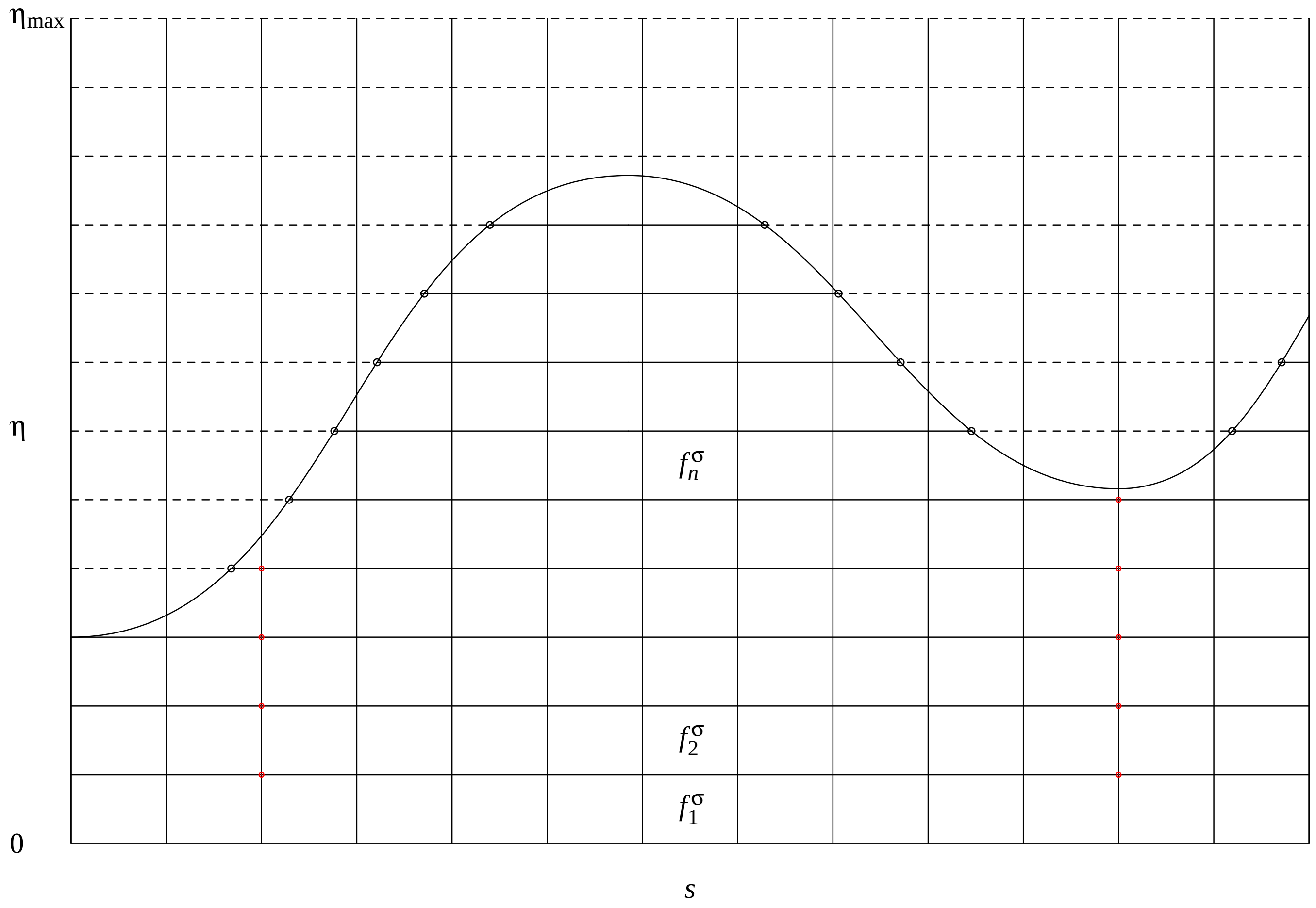
$$j_{\|} = \pi e B \sum_{\sigma=\pm 1} \int_0^{\infty} \mathrm{d}v\, v \int_0^{v^2/B} \mathrm{d}J_{\perp} \tilde{f}^{\sigma} = \frac{3c}{4B_0} \frac{\mathrm{d}p}{\mathrm{d}r} \frac{1}{\langle |\nabla\psi| \rangle} \hat{B} \int_0^{1/\hat{B}} \mathrm{d}\eta \left(\hat{f}^{+} - \hat{f}^{-} \right),$$

$$\lambda_{\|} = -j_{\|} \left(\frac{c\hat{B}}{B_0} \frac{\mathrm{d}p}{\mathrm{d}r} \right)^{-1} = -\frac{3}{4} \frac{1}{\langle |\nabla\psi| \rangle} \int_0^{1/\hat{B}} \mathrm{d}\eta \left(\hat{f}^{+} - \hat{f}^{-} \right)$$

$$\lambda_b \equiv \frac{\langle \lambda_{\|} B^2 \rangle}{\langle B^2 \rangle} = -\frac{3}{4} \lim_{L\to\infty} \int_0^{L} \frac{\mathrm{d}s}{\hat{B}} \left(\int_0^{L} \mathrm{d}s \hat{B} \right)^{-1} \left(\int_0^{L} \frac{\mathrm{d}s}{\hat{B}} |\nabla\psi| \right)^{-1} \Lambda(L)$$

$$\frac{\mathrm{d}\Lambda(s)}{\mathrm{d}s} = \hat{B} \int_0^{1/\hat{B}} \mathrm{d}\eta \left(\hat{f}^{+} - \hat{f}^{-} \right), \qquad \Lambda(0) = 0$$

Discretization over η - Scheme



$f_n^\sigma = \int_{\eta_{n-1}}^{\eta_n} d\eta \hat{f}^\sigma$	integrated flux densities for a band
$\eta_{n-1},\ \eta_n$	boundaries of band number n

Discretization over η

$$\sigma \frac{\partial f_n^\sigma}{\partial s} = -\frac{\kappa}{2}\left(\eta_n \left(\frac{\partial \hat{f}^\sigma}{\partial|\lambda|}\right)_n - \eta_{n-1}\left(\frac{\partial \hat{f}^\sigma}{\partial|\lambda|}\right)_{n-1}\right) + \left(\frac{|\lambda|\hat{V}_G}{\hat{B}}\right)_n - \left(\frac{|\lambda|\hat{V}_G}{\hat{B}}\right)_{n-1}$$

Taylor expansion over pitch λ around $\lambda_n = \lambda(s, \eta_n)$

$$\hat{f}^\sigma = f_0 + f_0'(|\lambda| - |\lambda_n|) + \frac{1}{2} f_0''(|\lambda| - |\lambda_n|)^2 + \frac{1}{6} f_0'''(|\lambda| - |\lambda_n|)^3$$

formal solution for third order finite difference approximation

$$\left(\frac{\mathrm{d}\hat{f}^\sigma}{\mathrm{d}|\lambda|}\right)_n \equiv \left.\frac{\mathrm{d}\hat{f}^\sigma}{\mathrm{d}|\lambda|}\right|_{\eta=\eta_n} = f_0' = \sum_{k=n-1}^{n+2} \mathcal{D}_{n,k} f_k^\sigma$$

third order conservative finite difference representation of the Lorentz collision operator

Discretized DKE

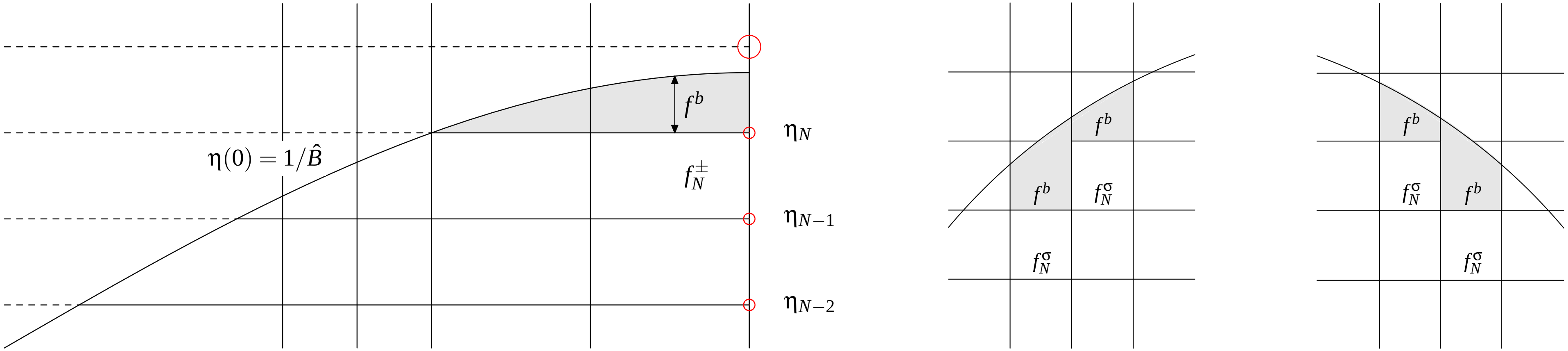
$$\frac{\partial f_n^\sigma}{\partial s} = \sum_{k=n-2}^{n+2} a_{n,k} f_k^\sigma + q_n$$

$$a_{n,k} = \frac{\sigma\kappa}{2}\begin{pmatrix} \eta_{n-1}\mathcal{D}_{n-1,n-2}, & k = n-2, \\ \eta_{n-1}\mathcal{D}_{n-1,k} - \eta_n\mathcal{D}_{n,k}, & n-1 \le k \le n+1, \\ -\eta_n\mathcal{D}_{n,n+2}, & k = n+2 \end{pmatrix},$$

$$q_n = \left(\frac{|\lambda|\hat{V}_G}{\hat{B}}\right)_n - \left(\frac{|\lambda|\hat{V}_G}{\hat{B}}\right)_{n-1}.$$

coupled set of linear ordinary differential equations for band-integrated flux densities

Boundary Problem

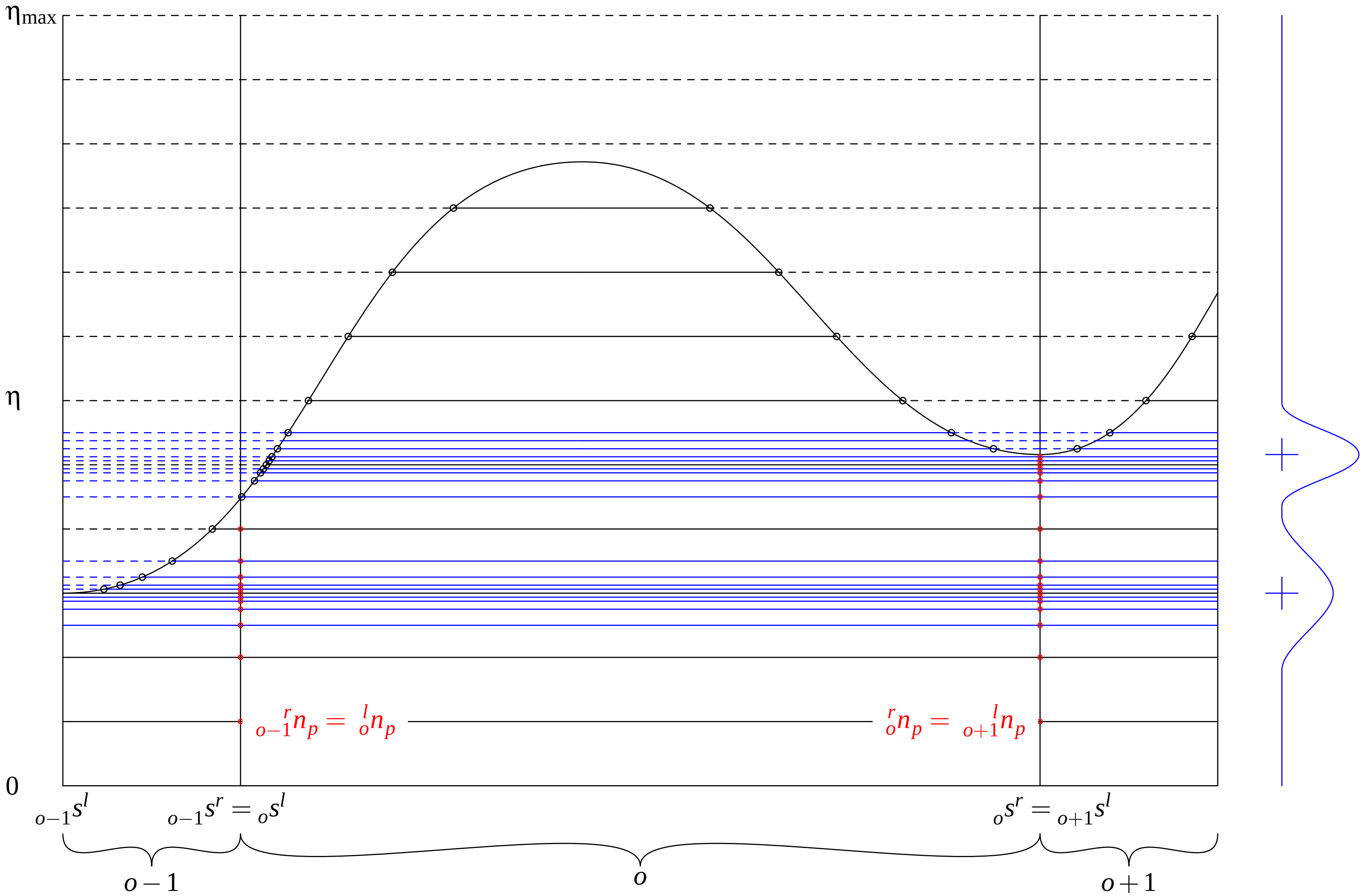


$$f^b = \int_{\eta_N}^{1/\hat{B}} d\eta\, \hat{f}^+ - \int_{\eta_N}^{1/\hat{B}} d\eta\, \hat{f}^- = \frac{2}{\hat{B}} \int_{-|\lambda_N|}^{|\lambda_N|} d\lambda\, \lambda f$$

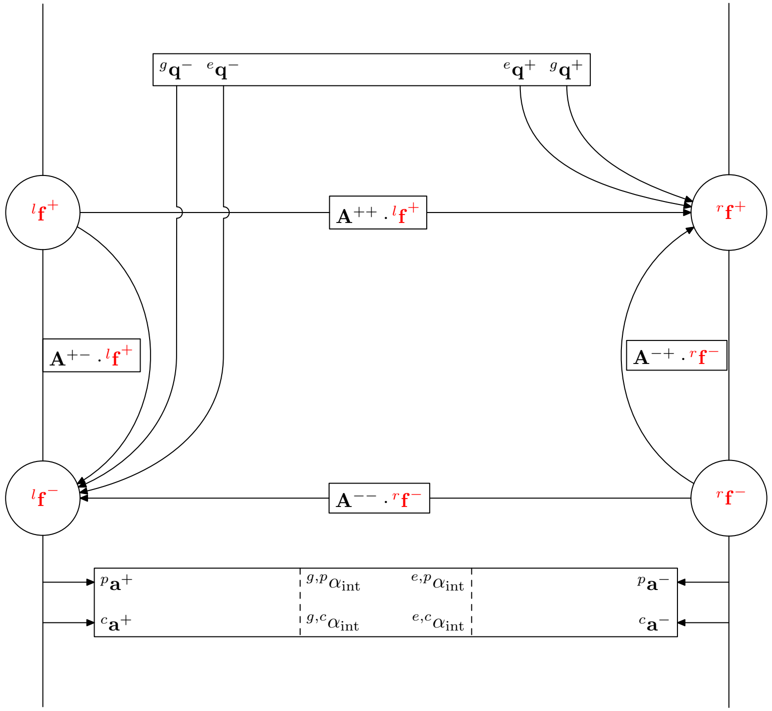
$$\frac{\partial f^b}{\partial s} = \frac{\kappa \eta_N}{2} \left(\left(\frac{\partial \hat{f}}{\partial \lambda} \right)_{\lambda=|\lambda_N|} - \left(\frac{\partial \hat{f}}{\partial \lambda} \right)_{\lambda=-|\lambda_N|} \right) - \left(\frac{2|\lambda| \hat{V}_G}{\hat{B}} \right)_{\lambda=|\lambda_N|}$$

Flux density integrated over boundary layer

Placing of Levels - Introduction of Ripples



Propagator



${}^{l}_{o}\mathbf{f}^{+}\ ,\ {}^{l}_{o}\mathbf{f}^{-}\ ,\ {}^{r}_{o}\mathbf{f}^{+}\ ,\ {}^{r}_{o}\mathbf{f}^{-}$	level integrated phase space flux density
${}^{g}_{o}\mathbf{q}^{-}\ ,\ {}^{g}_{o}\mathbf{q}^{+}\ ,\ {}^{e}_{o}\mathbf{q}^{-}\ ,\ {}^{e}_{o}\mathbf{q}^{+}$	sources from inside
${}^{g,p}_{o}\alpha_{int}\ ,\ {}^{e,p}_{o}\alpha_{int}\ ,\ {}^{g,c}_{o}\alpha_{int}\ ,\ {}^{e,c}_{o}\alpha_{int}$	mfl integrals of particle flux and current
${}^{p}_{o}\mathbf{a}^{+}\ ,\ {}^{p}_{o}\mathbf{a}^{-}\ ,\ {}^{c}_{o}\mathbf{a}^{+}\ ,\ {}^{c}_{o}\mathbf{a}^{-}$	distribution of flux (current) production (ext)
${}_{o}\mathbf{A}^{++}\ ,\ {}_{o}\mathbf{A}^{--}\ ,\ {}_{o}\mathbf{A}^{+-}\ ,\ {}_{o}\mathbf{A}^{-+}$	convolution matrices

Propagator - Additional Formulas

Convolution plus sources

$$
\begin{aligned}
{}^{r}_{o}\mathbf{f}^{+} &= {}_{o}\mathbf{A}^{++} \cdot {}^{l}_{o}\mathbf{f}^{+} + {}_{o}\mathbf{A}^{-+} \cdot {}^{r}_{o}\mathbf{f}^{-} + {}^{g}_{o}\mathbf{q}^{+} + {}^{e}_{o}\mathbf{q}^{+} \\
{}^{l}_{o}\mathbf{f}^{-} &= {}_{o}\mathbf{A}^{--} \cdot {}^{r}_{o}\mathbf{f}^{-} + {}_{o}\mathbf{A}^{+-} \cdot {}^{l}_{o}\mathbf{f}^{+} + {}^{g}_{o}\mathbf{q}^{-} + {}^{e}_{o}\mathbf{q}^{-}
\end{aligned}
$$

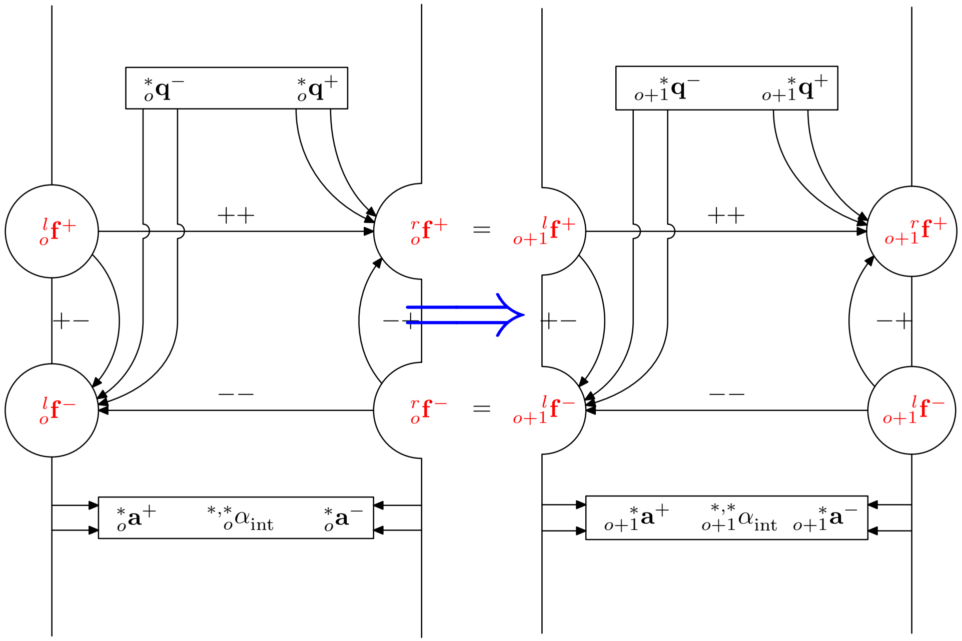
Field line integrals of flux and current are expressed through efficiencies (external, total)

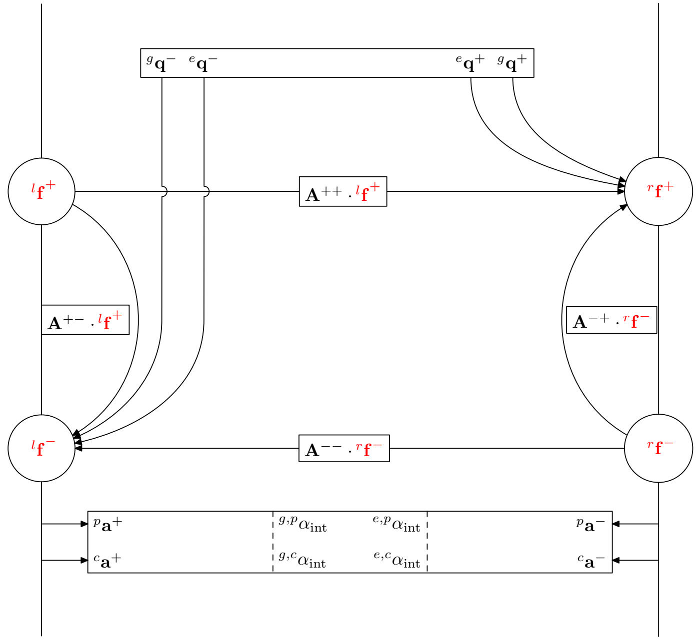
$$
\begin{aligned}
{}^{p}_{o}\alpha_{ext} &= {}^{p}_{o}\mathbf{a}^{+} \cdot {}^{l}_{o}\mathbf{f}^{+} + {}^{p}_{o}\mathbf{a}^{-} \cdot {}^{r}_{o}\mathbf{f}^{-} \\
{}^{c}_{o}\alpha_{ext} &= {}^{c}_{o}\mathbf{a}^{+} \cdot {}^{l}_{o}\mathbf{f}^{+} + {}^{c}_{o}\mathbf{a}^{-} \cdot {}^{r}_{o}\mathbf{f}^{-} \\
{}^{p}_{o}\alpha_{tot} &= {}^{p}_{o}\alpha_{ext} + {}^{g,p}_{o}\alpha_{int} + {}^{e,p}_{o}\alpha_{int} \\
{}^{c}_{o}\alpha_{tot} &= {}^{c}_{o}\alpha_{ext} + {}^{g,c}_{o}\alpha_{int} + {}^{e,c}_{o}\alpha_{int}
\end{aligned}
$$

Joining of Propagators

Propagators have group properties

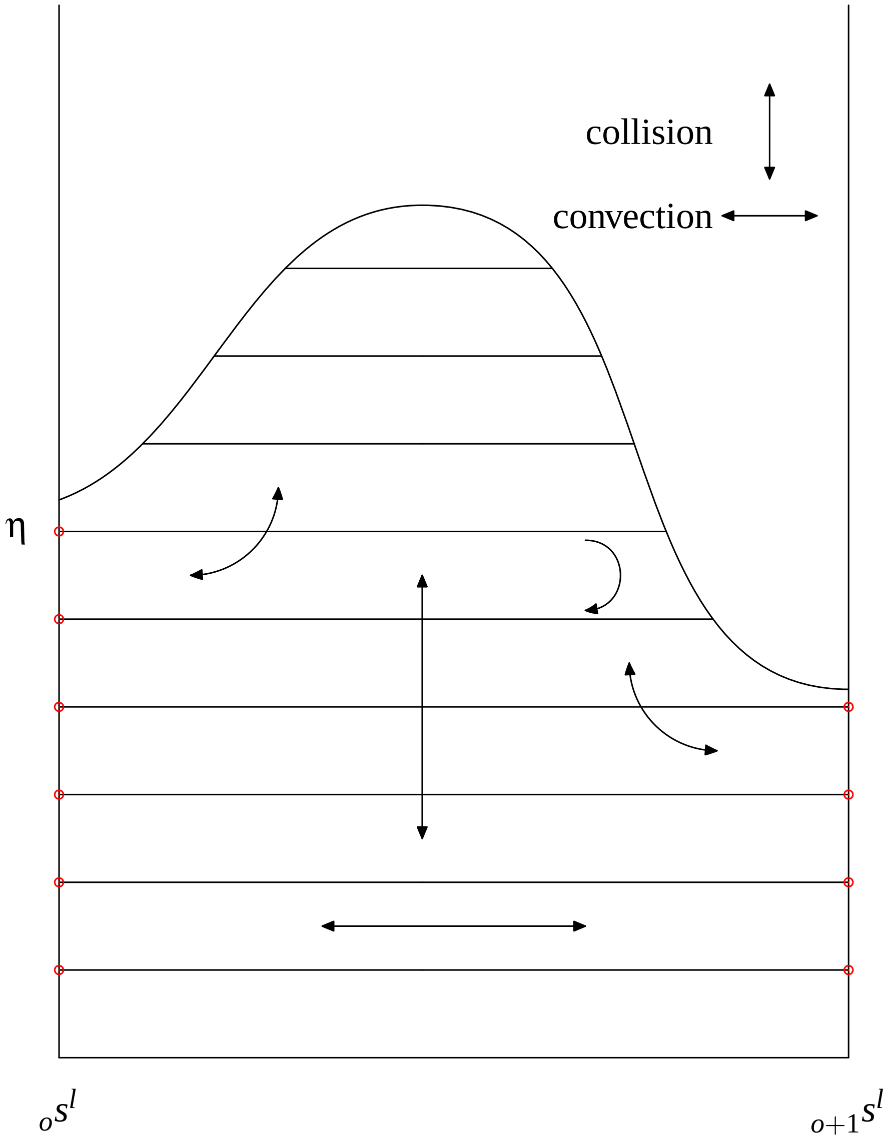
$$ {}_1P * {}_2P = {}_{1,2}P \quad , \quad {}_1P * ({}_2P * {}_3P) = ({}_1P * {}_2P) * {}_3P $$



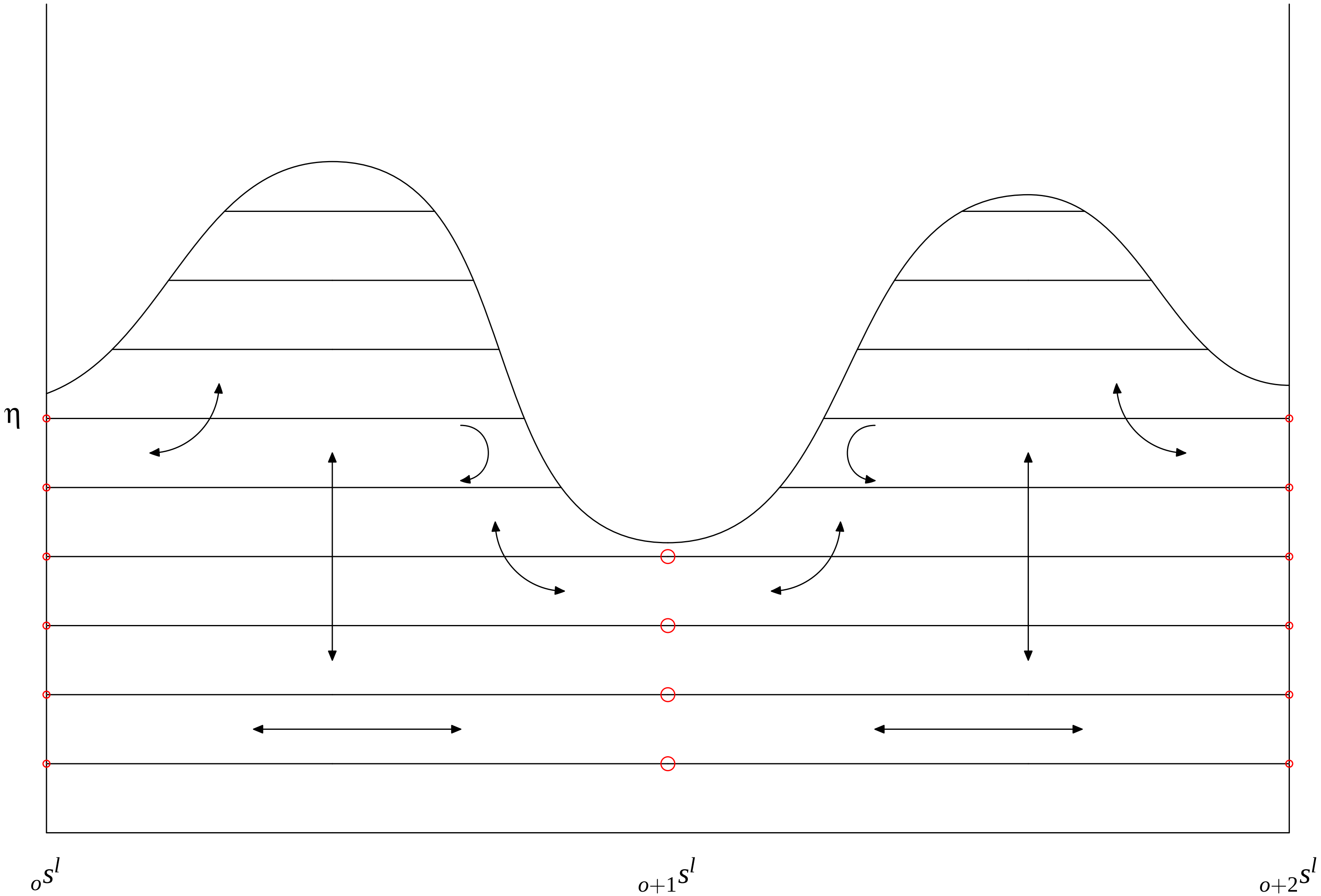


Numerics
- solving systems of linear equations
- convolution of matrices
- band structure

Propagator Visualization - 1



Propagator Visualization - 2



Back to Solution within the Ripple - Renormalization

General solution in $+$ $(\lambda > 0)$ and $-$ $(\lambda < 0)$ half-spaces

$$\mathbf{f}(s) = \begin{pmatrix} \mathbf{f}^{+}(s) \\ \mathbf{f}^{-}(s) \end{pmatrix} = \begin{pmatrix} f_i^{+}(s) \\ f_i^{-}(s) \end{pmatrix}$$

- Boundary layer included on negative half-space (free choice)

- Integration of DKE in positive direction
  one does not want to go forward and backward in RK
  - half-space with $\lambda > 0$: Diffusion
    dispersing solution
  - half-space with $\lambda < 0$: Anti-Diffusion
    peaking solution $\Rightarrow$ numerically unstable

- Solution Renormalization

Renormalization - Start

DKE Solver ($\Longrightarrow$) Backward Boundary condition at first step

$$
\begin{array}{lcl|}
{}_{(1)}g^{+}_{ik}(s_0) = 0 & \Longrightarrow & {}_{(1)}g^{+}_{ik}(s_1) \\
{}_{(1)}g^{-}_{ik}(s_0) = \delta_{ik} & \Longrightarrow & {}_{(1)}g^{-}_{ik}(s_1) \\
\hline
{}_{(1)}f^{+}_{i}(s_0) = {}^{l}f^{+}_{i} & \Longrightarrow & {}_{(1)}f^{+}_{i}(s_1) \\
{}_{(1)}f^{-}_{i}(s_0) = 0 & \Longrightarrow & {}_{(1)}f^{-}_{i}(s_1) \\
\hline
f^{+}_{i}(s_0) = {}^{l}f^{+}_{i} & & \\
f^{-}_{i}(s_0) = {}_{(1)}\beta_i & \Longleftarrow &
\end{array}
$$

Green's function ${}_{(n)}g^{\pm}_{ik}$ and shifted solution ${}_{(n)}f^{\pm}_{i}$ in renormalization interval n

Renormalization - Intermediate

Forward | Backward | Boundary condition at intermediate boundary s_n

$$
\begin{array}{lrcl}
{}_{(n)}g^+_{ij}(s_n) \;| & {}_{(n)}g^+_{ij}(s_n)\,{}_{(n)}C_{jk} & = & {}_{(n+1)}g^+_{ij}(s_n) \;\Longrightarrow \\
{}_{(n)}g^-_{ij}(s_n) \;| & {}_{(n)}g^-_{ij}(s_n)\,{}_{(n)}C_{jk} = \delta_{ik} & = & {}_{(n+1)}g^-_{ij}(s_n) \;\Longrightarrow
\end{array}
$$

$$
\begin{array}{lrcl}
{}_{(n)}f^+_{i}(s_n) \;| & {}_{(n)}f^+_{i}(s_n) - {}_{(n)}g^+_{ik}(s_n)\,{}_{(n)}\alpha_k & = & {}_{(n+1)}f^+_{i}(s_n) \;\Longrightarrow \\
{}_{(n)}f^-_{i}(s_n) \;| & {}_{(n)}f^-_{i}(s_n) - {}_{(n)}g^-_{ik}(s_n)\,{}_{(n)}\alpha_k = 0 & = & {}_{(n+1)}f^-_{i}(s_n) \;\Longrightarrow
\end{array}
$$

$$
{}_{(n)}\alpha_k = {}_{(n)}C_{ki}\,{}_{(n)}f^-_i(s_n) \;\Longrightarrow
$$

$$
{}_{(n)}\beta_k = {}_{(n)}C_{kj}\,{}_{(n+1)}\beta_j - {}_{(n)}\alpha_k \;\Longleftarrow
$$

$$
f^+_i(s_n) = {}_{(n)}f^+_i(s_n) + {}_{(n)}g^+_{ik}(s_n)\,{}_{(n)}\beta_k \;\Longleftarrow
$$

$$
f^-_i(s_n) = {}_{(n+1)}\beta_i \;\Longleftarrow
$$

Renormalization - Final

Forward | Backward | Boundary condition at s_N

$${}_{(N)}g^{+}_{ij}(s_N) \quad |$$

$${}_{(N)}g^{-}_{ij}(s_N) \quad | \qquad {}_{(N)}g^{-}_{ij}(s_N)\, {}_{(N)}C_{jk} = \delta_{ik}$$

$${}_{(N)}f^{+}_{i}(s_N) \quad |$$

$${}_{(N)}f^{-}_{i}(s_N) \quad | \qquad {}_{(N)}f^{-}_{i}(s_N) - {}_{(N)}g^{-}_{ik}(s_N)\, {}_{(N)}\alpha_k = 0$$

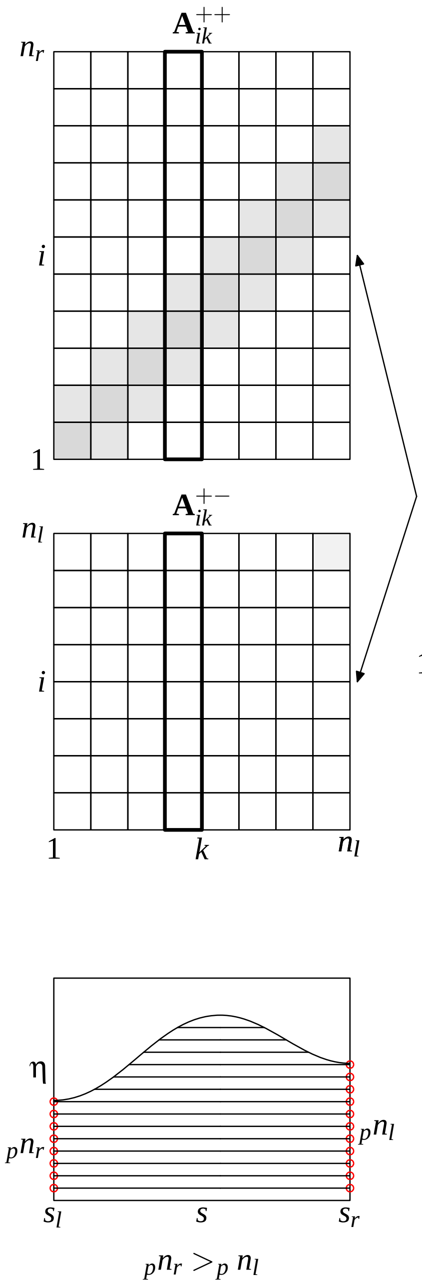
$${}_{(N)}\alpha_k = {}_{(N)}C_{ki}\, {}_{(N)}f^{-}_{i}(s_N)$$

$${}_{(N)}\beta_k = {}_{(N)}C_{ki}\, {}^{r}f^{-}_{i} - {}_{(N)}\alpha_k$$

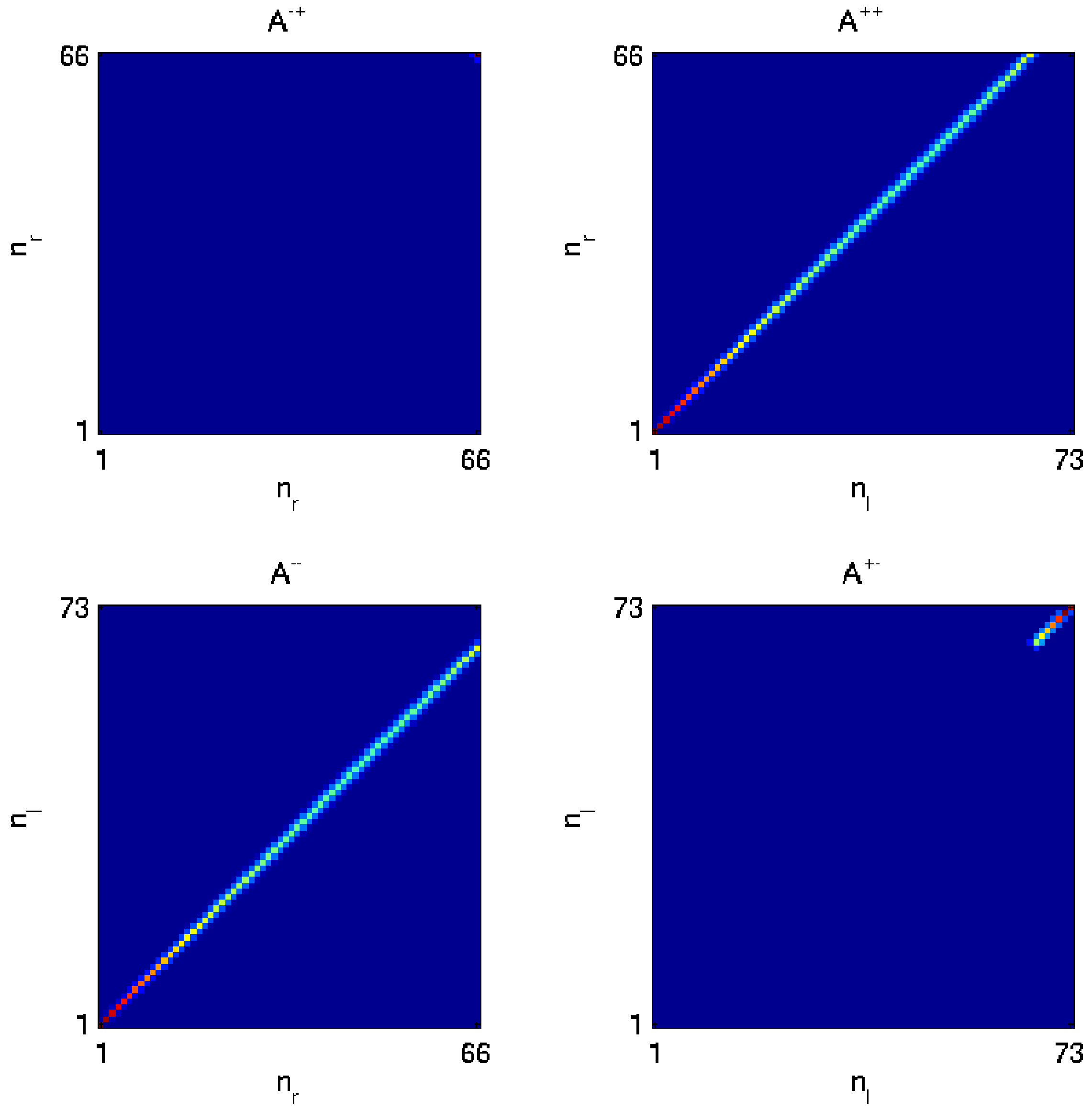
$$f^{+}_{i}(s_N) = {}_{(N)}f^{+}_{i}(s_N) + {}_{(N)}g^{+}_{ik}(s_N)\, {}_{(N)}\beta_k$$

$$f^{-}_{i}(s_n) = {}^{r}f^{-}_{i}$$

Constructing the Solution

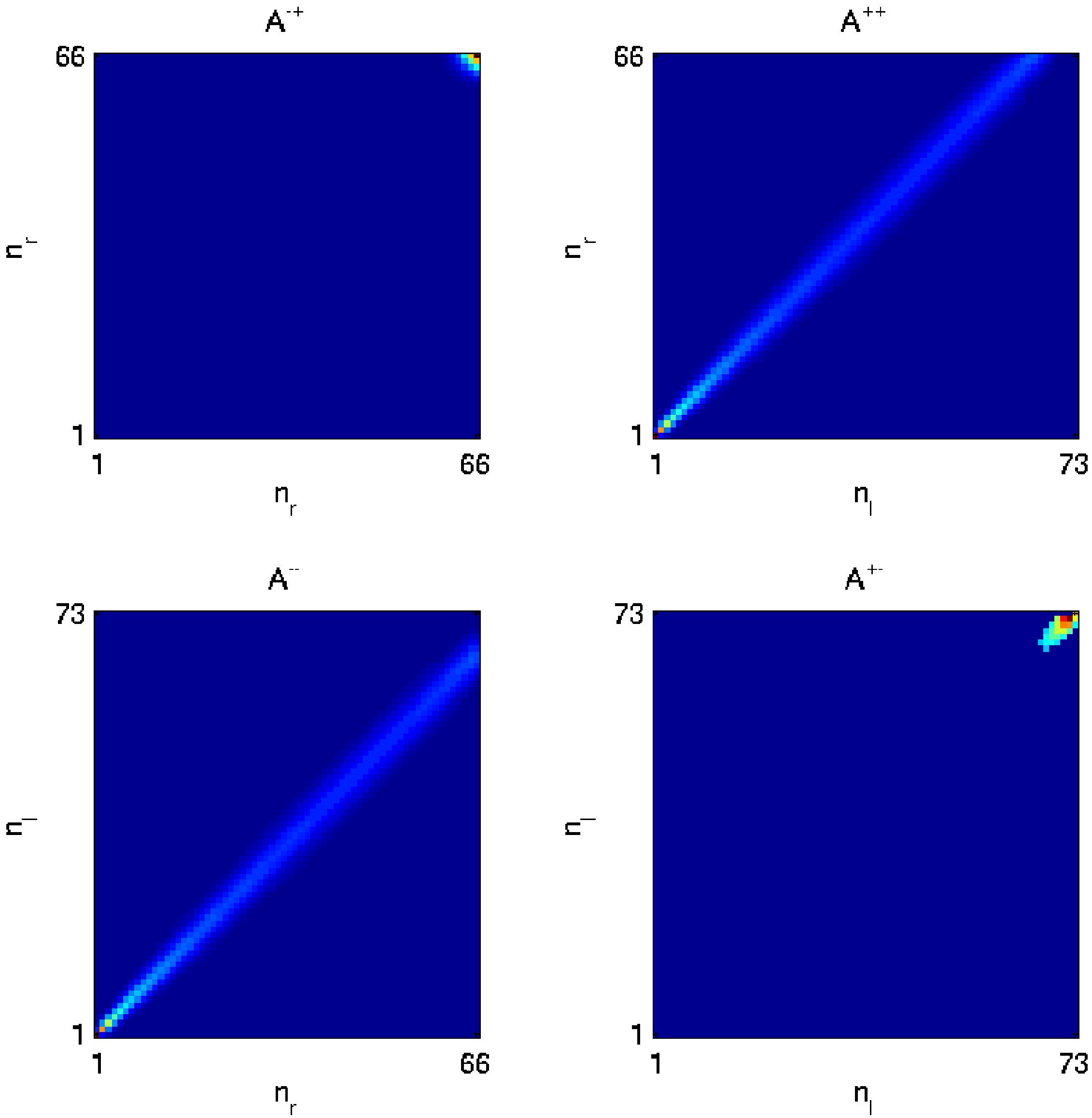


Solution within the Ripple - Low Collision



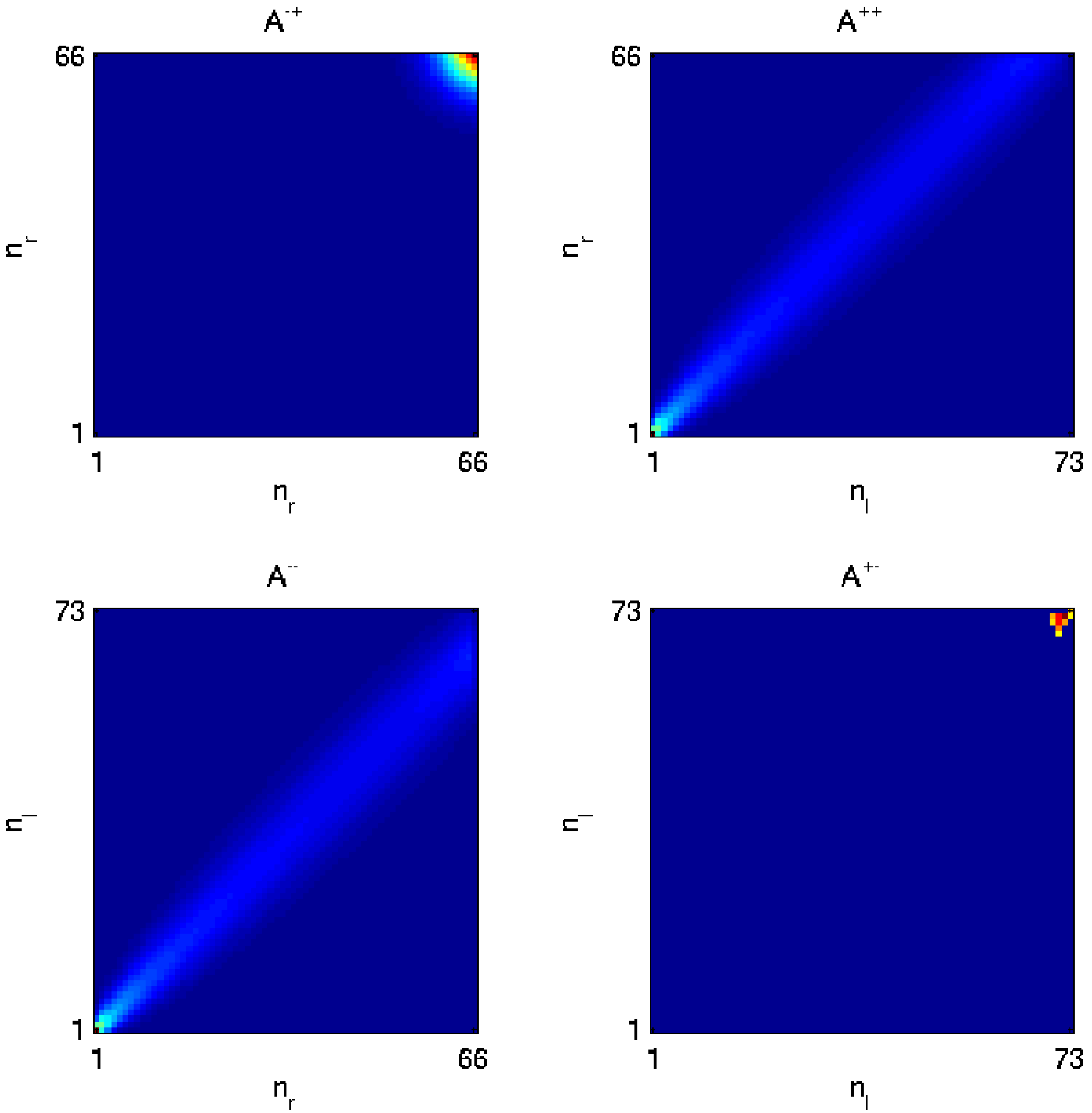
$$\kappa = 1 \cdot 10^{-3}$$

Solution within the Ripple - Medium Collision



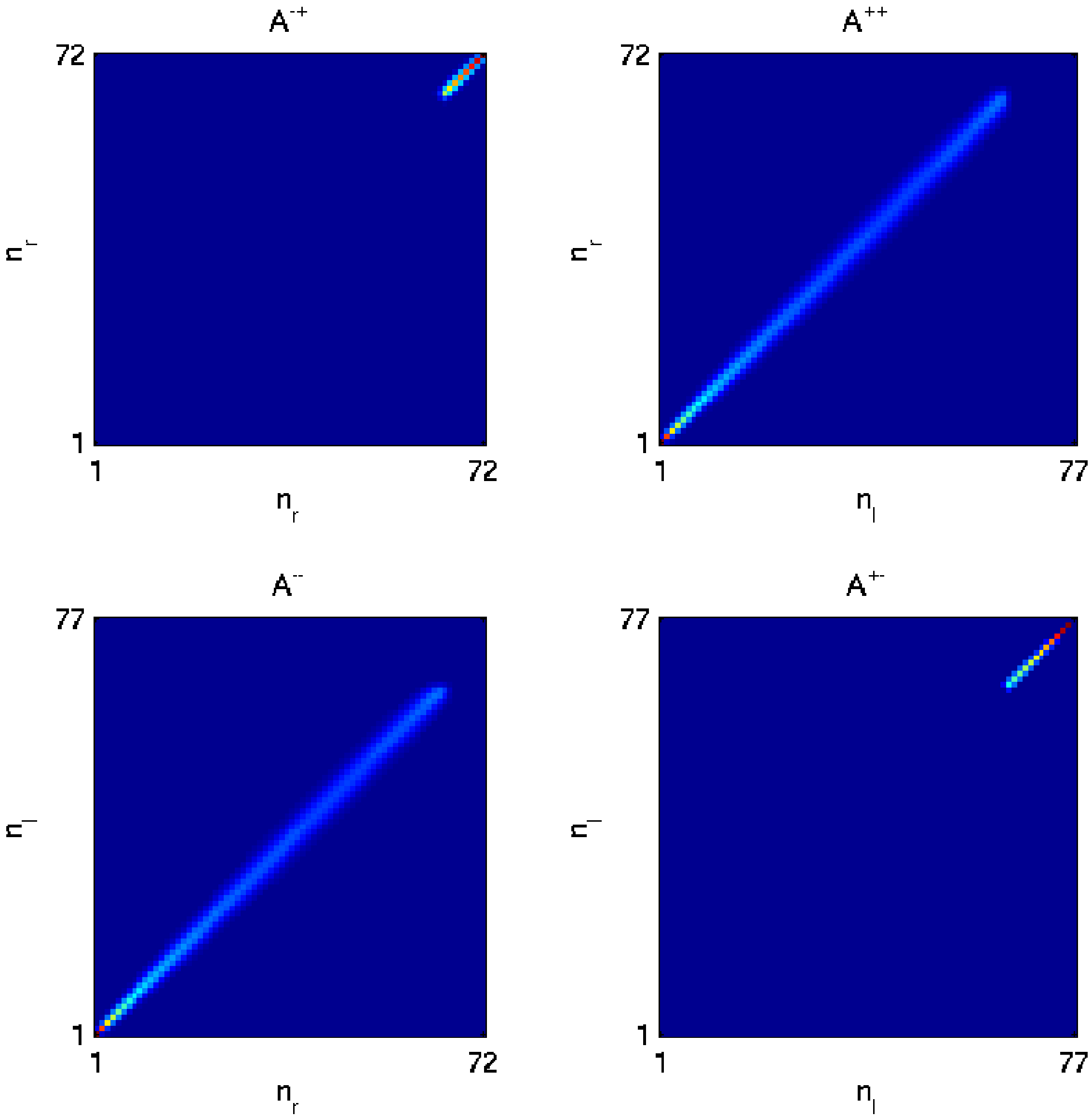
$$\kappa = 1 \cdot 10^{-2}$$

Solution within the Ripple - High Collision



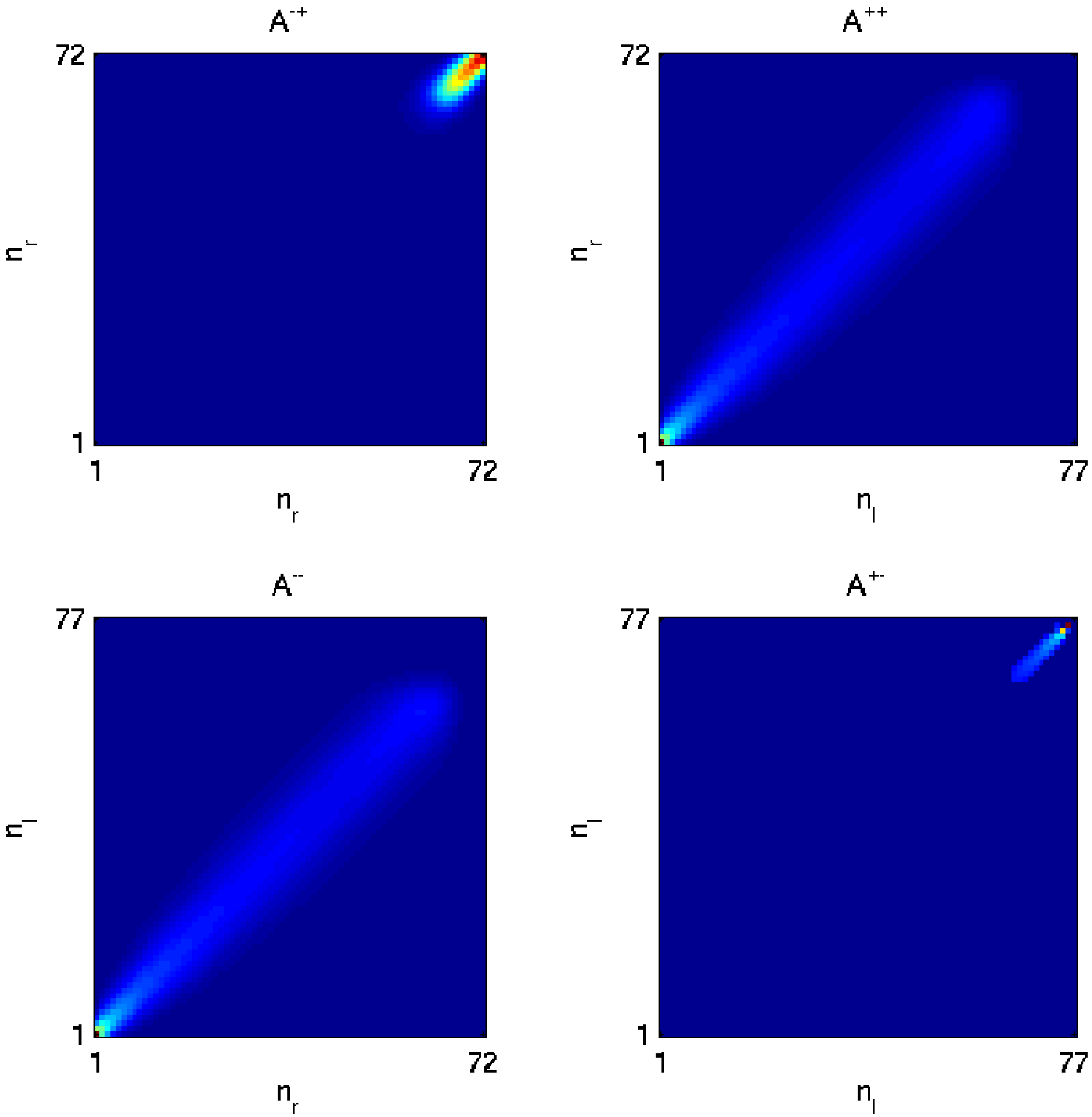
$$\kappa = 5 \cdot 10^{-2}$$

Solution for Joined Ripple - Low Collision



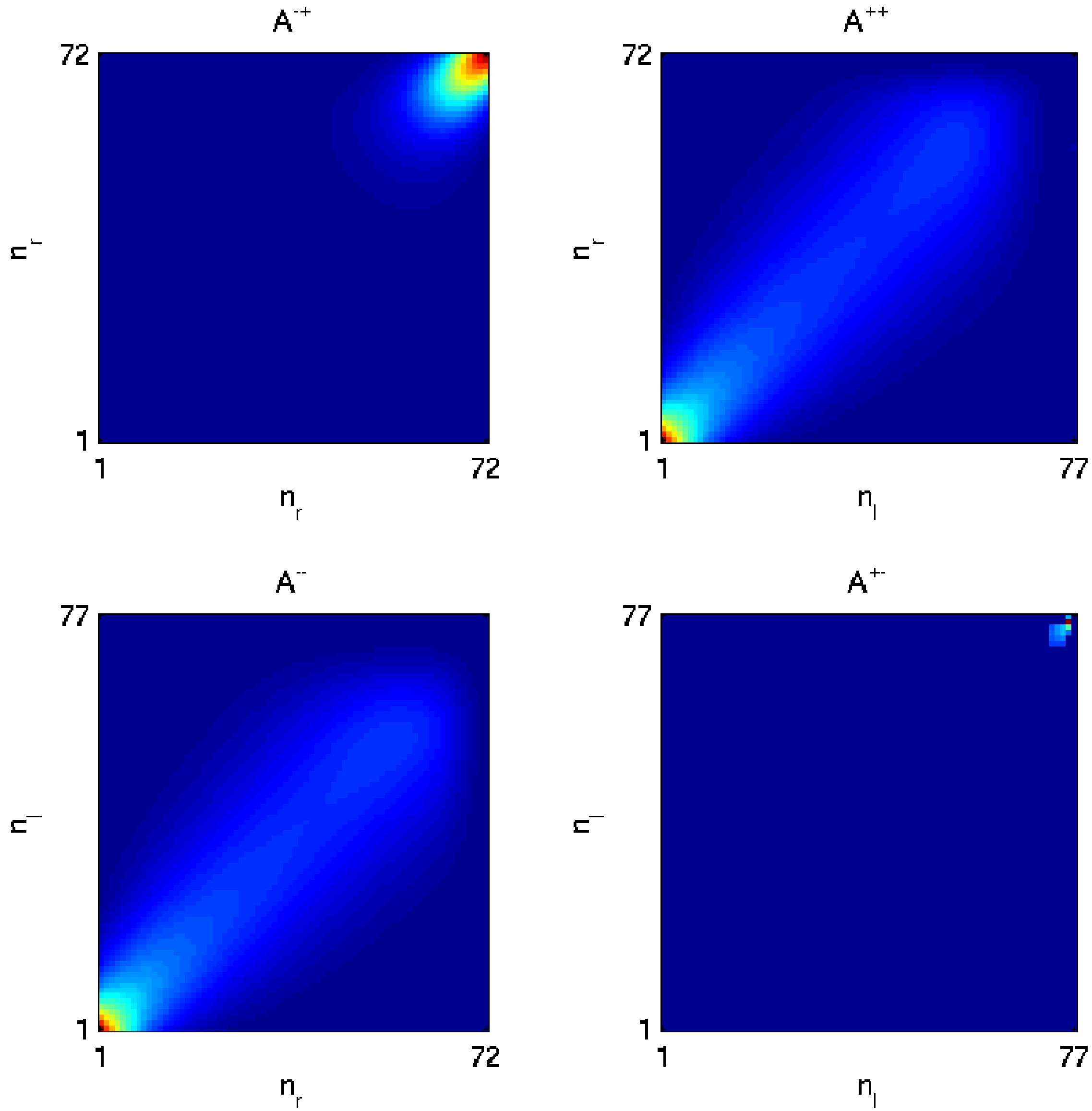
$$\kappa = 1 \cdot 10^{-3}$$

Solution for Joined Ripple - Medium Collision



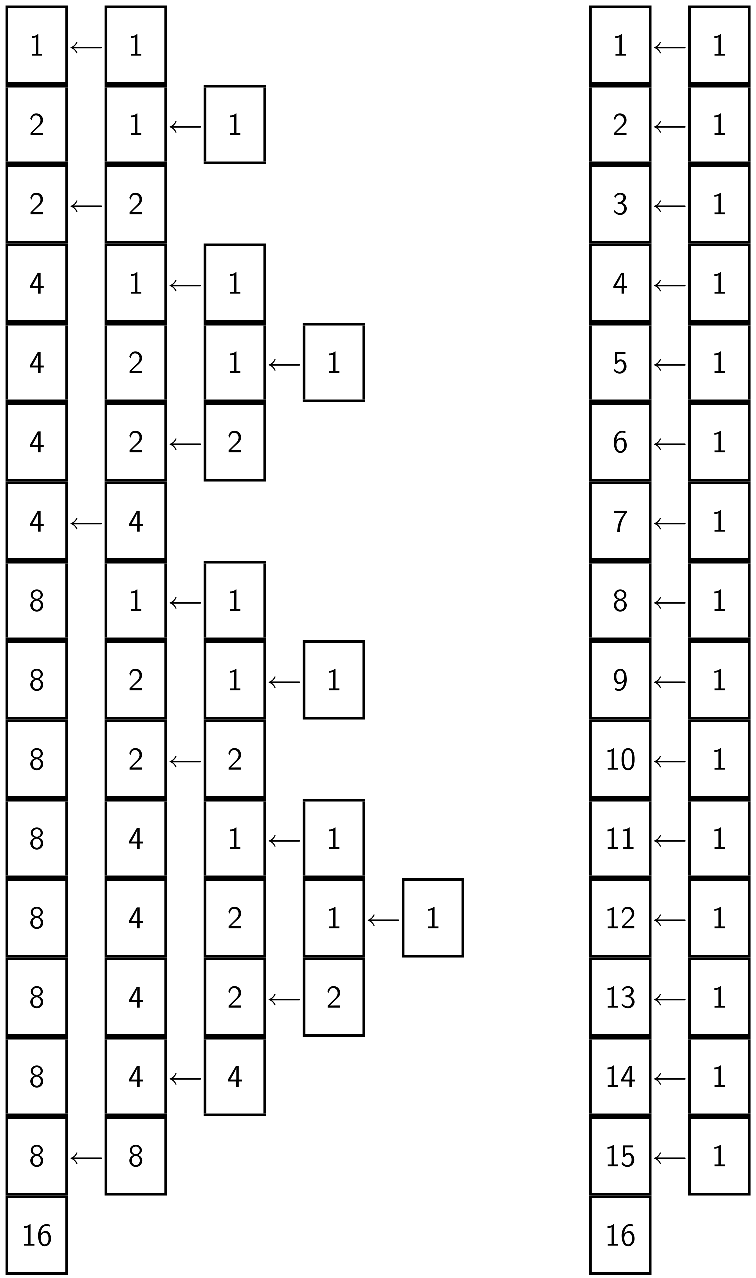
$$\kappa = 1 \cdot 10^{-2}$$

Solution for Joined Ripple - High Collision



$$\kappa = 5 \cdot 10^{-2}$$

Binary Joining



$$n_h = [\sqrt{({}_o n_h)^2 + ({}_{o+1} n_h)^2}]$$

Solution of the drift kinetic equation

Drift kinetic equation:

$$\mathcal{L}_D(f_a) = \mathcal{L}_C(f_a, f_b) + Q$$

f_a	distribution function of particle species a
$\mathcal{L}_D$	describes particle motion in various electric and magnetic fields
$\mathcal{L}_C$	Coulomb collision operator
Q	source term

Full linearized Coulomb collision operator:

$$\mathcal{L}_C(f_{a0} + f_{a1}, f_{b0} + f_{b1}) \cong \mathcal{L}_C(f_{a0}, f_{b0}) + \mathcal{L}_C(f_{a1}, f_{b0}) + \mathcal{L}_C(f_{a0}, f_{b1})$$

f_{a0}, f_{b0}	Maxwellian distribution functions
f_{a1}, f_{b1}	correction terms $(f_1/f_0 \ll 1)$
$\mathcal{L}_C(f_{a0}, f_{b0})$	is zero if both Maxwellians have the same temperature

f_{a1} is expanded in terms of a complete set of orthogonal velocity-space functions:

$$f_{a1}(\mathbf{r},\mathbf{v},t) = \sum_{l=0}^{\infty}\sum_{n=0}^{\infty} c_{ln}^{(a)}(\mathbf{r},t) B_{ln}(\mathbf{x_a}) f_{a0}$$

$c_{ln}^{(a)}$	expansion coefficients
B_{ln}	Burnett functions
$\mathbf{x_a} = \mathbf{v}/v_{ta}$	normalized particle velocity

Burnett functions:

$$B_{ln}(\mathbf{x_a}) = x_a^l L_n^{(l+1/2)}(x_a^2) P_l(\cos\theta)$$

$L_n^{(l+1/2)}$	associated Laguerre polynomials
P_l	Legendre polynomials
θ	polar angle of $\mathbf{v}$ in a spherical coordinate system

Solution to the DKE:

- substitution of the expansion for f_{a1} into the DKE
- multiplication of the DKE on the left by the basis function $B_{l'n'}$
- integration over $\mathbf{v}$
- DKE is converted into an infinite set of linear equations for c_{ln}

$$\sum_{l=0}^{\infty}\sum_{n=0}^{\infty} c_{ln}^{(a)} \left(\mathcal{L}^{D}_{l'n',ln} - \mathcal{L}^{C}_{l'n',ln}\right) = Q_{l'n'}$$

$\mathcal{L}_{i'j',ij}$ matrix elements

Matrix elements (ME) of the linearized Coulomb operator: (see, e. g. [1])

$$\mathcal{L}^{C}_{l'n',ln} = M^{(l)}_{n',n} + N^{(l)}_{n',n}$$

differential part: $$M^{(l)}_{n',n} = \int \mathrm{d}\mathbf{v} B_{l'n'} \mathcal{L}_C(B_{ln} f_{a0}, f_{b0})$$

integral part: $$N^{(l)}_{n',n} = \int \mathrm{d}\mathbf{v} B_{l'n'} \mathcal{L}_C(f_{a0}, B_{ln} f_{b0})$$

- ME can be computed by means of a generated function technique [2]
- generating functions for the ME are governed by recursion relations
- thus, fast numerical evaluation of the ME is possible

Radial Electric Field

- Approximate the cross field convection (rotation) term with the help of finite-difference scheme over θ_0
- Generalize renormalization procedure to allow for field maxima within the ripple
- Solve the coupled (cross field convection) system of ODEs for all field lines which start at $\phi = 0$,
- Integrate them to the end of a field period
- Apply the periodicity condition
- Sparse matrices, band-block structure
- Standard way - HARD PROBLEM: Adaptive grid in phase space
- Alternative - 2-D Propagators - wait for NEO-3

References

[1] S. K. Wong, *Phys. Fluids* **28**, 1695 (1985).

[2] S. I. Braginskii, *Sov. Phys. JETP* **6**, 358 (1958).