Numerical radiative transfer II

Contents

- TR3D
  - discretization
  - mean intensity approach
  - pros and cons
- D3NEBEL
  - 3D through a set of independent rays
  - discretization and integration along rays

Numerical techniques in TR3D

The radiative transfer equation in TR3D

$$\underline{n} \cdot \nabla_x I^\nu = \eta^\nu - \underbrace{(\kappa^\nu + \lambda^\nu)}_{\chi} I^\nu + \lambda^\nu \int_{S^2} d\Omega\, I^\nu$$

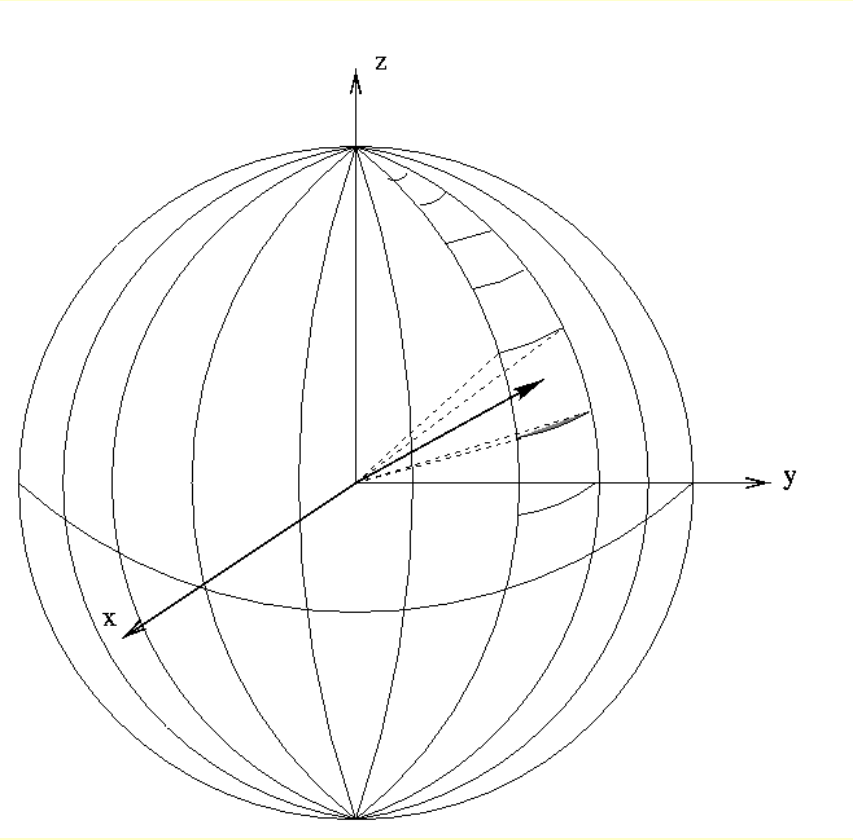
$$n \in S^2,\ I^\nu = I^\nu(\boldsymbol{x}, \boldsymbol{n})$$

I^ν: specific (directed) intensity
η: emission coefficient
κ: absorption coefficient
λ: scattering coefficient

x: position in space
n: direction of propagation
S^2: unite sphere in 3D

Discretization of ordinate space

- Use equidistant discretization
  of [0,2π) and [0,π]
- Replace $\int d\Omega\, I$ by quadrature sum



$$n^m \nabla_x I^m(x) + \chi^m I^m(x) =$$

$$\lambda(x) \sum_{k=1}^{M} c_k I^k(x) + \eta^m(x)$$

$$\forall m, \forall \nu$$

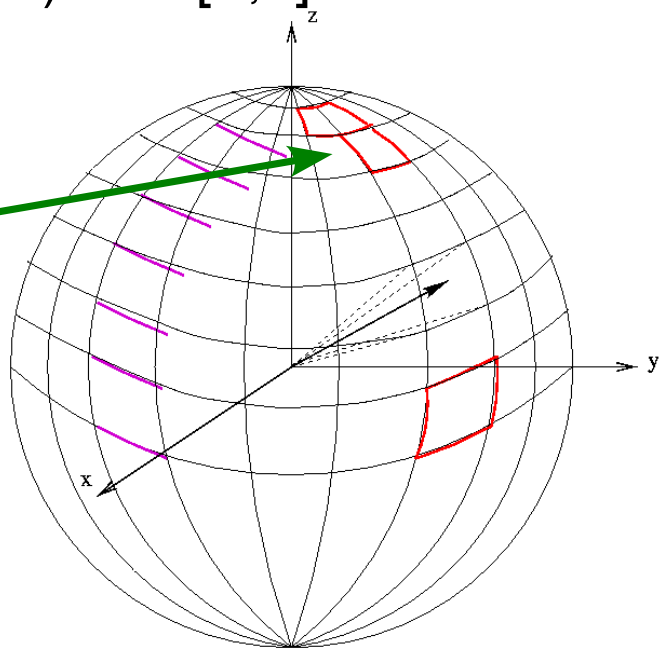
m=discrete ordinate directions

c_k = integration weights

$$\sum_{k=1}^{M} c_k = 1$$

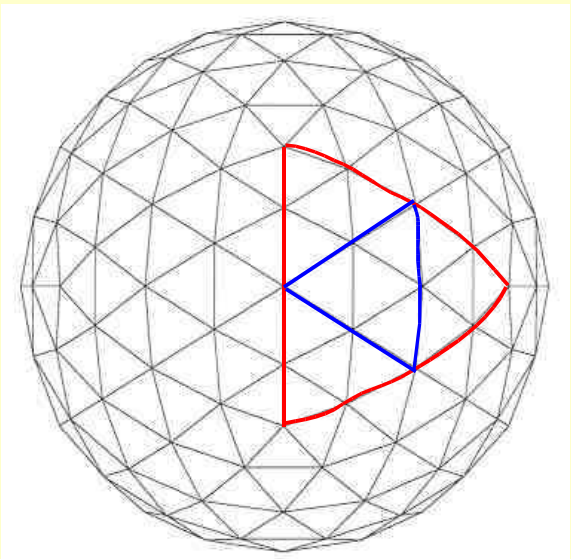
Variations

Problem with equidistant discretization of [0,2π) and [0,π]:
Concentration of ordinates around the poles



Possible solutions:

i) Use equidistant discretization
of [0,2π) and [0,π], but omit part
of the ordinates as the poles
are approached
Pro: rather flexible # of ordinates
Con: angle elements of variable size



ii) Define ordinate directions using
an icosahedron
Pro: angle elements of equal size
Con: # ordinates must be a multiple of 24

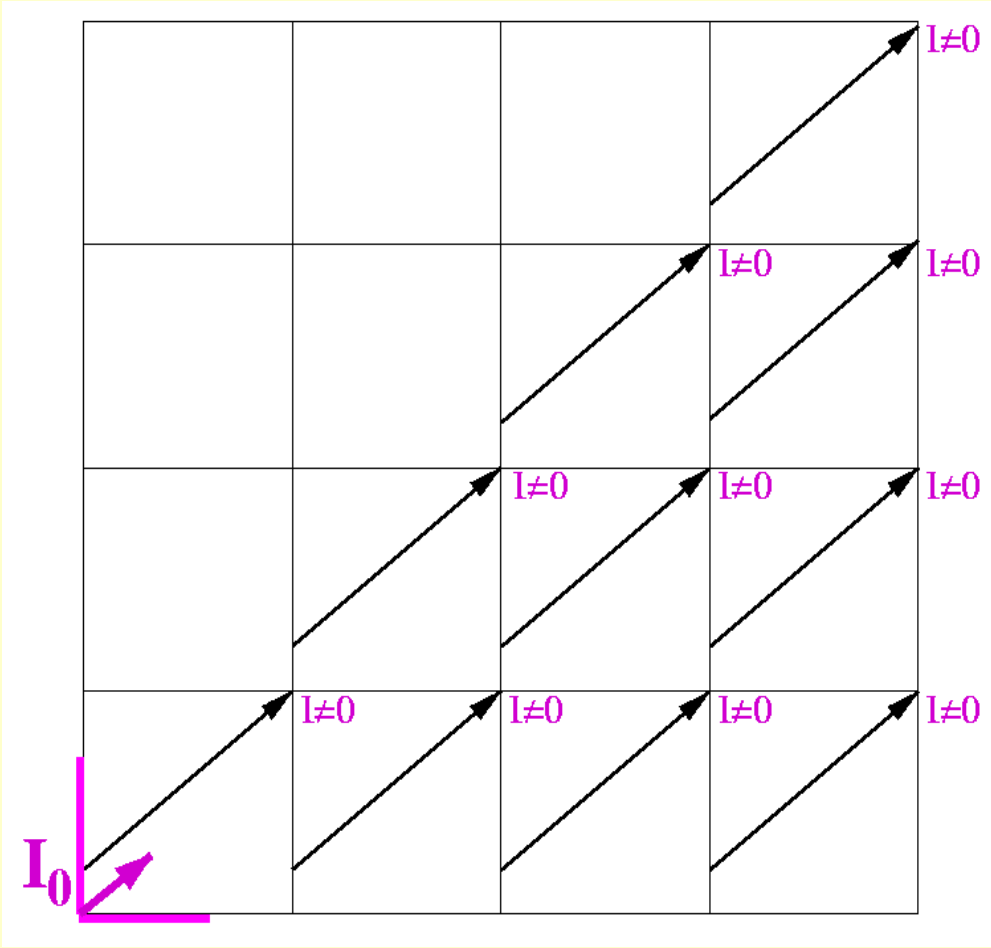
Spatial discretization:

Use:

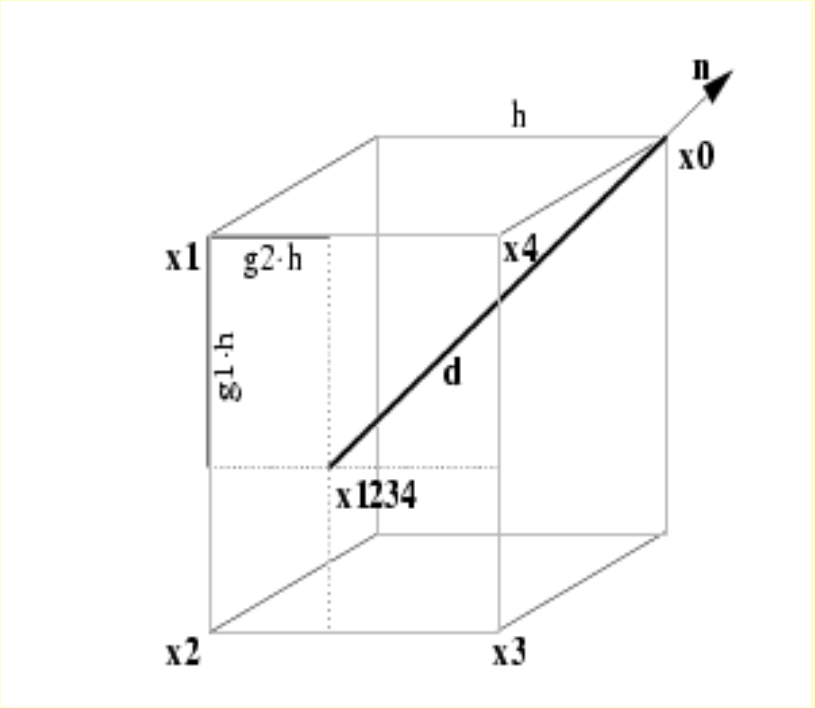
- equidistant Cartesian grid
- short characteristics
- 1st order approximation to directional derivative $n_m \nabla_x I^m$

Remember:

Short characteristics $\Rightarrow$ discrete expression for specific intensity at point x_0 contains only data from immediately neighbouring points to x_0



1st order approximation to directional derivative $n_m \nabla_x I^m$:



$$n^m \nabla_x I^m(x_0) = I_0^m - \frac{I_{1234}^m}{d} + O(h)$$

$$= I_0^m - I_1^m(1 - g_1 - g_2 + g_1 g_2) d^{-1} -$$
$$I_2^m(g_1 - g_1 g_2) d^{-1} - I_3^m(g_1 g_2) d^{-1} -$$
$$I_4^m(g_2 - g_1 g_2) d^{-1} + O(h)$$

Continuous form of transfer equation for one frequency ν and direction n

$$\underline{n} \cdot \underline{\nabla}_x I^\nu + \underbrace{(\kappa^\nu + \lambda^\nu)}_{\chi^\nu} I^\nu = \lambda^\nu \int d\Omega\, I^\nu + \eta^\nu$$

now has become a linear system of equations (for one discrete ν and m)

$$T_h^m I_h^m = L_h \sum_{k=1}^{M} c^k I_h^k + \eta_h^m$$

where: - I_h^m is a vector of length N_h (I^m at each of the N_h spatial grid points)

- T_h^m is a lower triangular matrix of rank N_h
  ($n_m \nabla_x I^m + \chi$ at each point x)
- L_h is a diagonal matrix of rank N_h (λ at each point x)
- η^m is a vector of length nnode

Such a system of equations has to be soved for each discrete direction m and each discrete frequency

Mean intensity approach

Basic idea: S.Turek, Impact of computation in science and engineering, vol.5, p.201

The discretized radiative transfer problem to be solved consists of

$M * N_\nu$ linear systems of equation

To each system belongs a matrix of rank N_h

M = number of ordinate directions

N_ν = number of frequency

N_h = number of spatial grid points

Instead of solving the transfer equation for one direction m after another, and iterating over directions, reformulate the discretized problem in terms of the angle integrated mean intensity

$$T_h^m I_h^m = L_h \sum_{k=1}^{M} c^k I_h^k + \eta_h^m$$

$$\Leftrightarrow \quad I_h^m = (T_h^m)^{-1} L_h \sum_{k=1}^{M} c^k I_h^k + (T_h^m)^{-1} \eta_h^m$$

$$\Leftrightarrow \quad \underbrace{\sum_{m=1}^{M} c^m I_h^m}_{J_h} = \underbrace{\sum_{m=1}^{M} c^m (T_h^m)^{-1}}_{T_h} L_h \underbrace{\sum_{k=1}^{M} c^k I_h^k}_{J_h} + \underbrace{\sum_{m=1}^{M} c^m (T_h^m)^{-1} \eta_h^m}_{F_h}$$

$$\Leftrightarrow \quad J_h = T_h L_h J_h + F_h$$

$$\Leftrightarrow \quad (1_h - T_h L_h) J_h = F_h$$

Have now one system of equations for the mean intensity instead of one system per ordinate direction

Inversion of T_h^m and renumbering

Reformulation of transfer equations for each specific intensity I^m_h into a system equation for J_h requires inversion of T^m_h:

$$T_h^m I_h^m = L_h \sum_{k=1}^{M} c^k I_h^k + \eta_h^m$$

$$I_h^m = (T_h^m)^{-1} L_h \sum_{k=1}^{M} c^k I_h^k + (T_h^m)^{-1} \eta_h^m$$

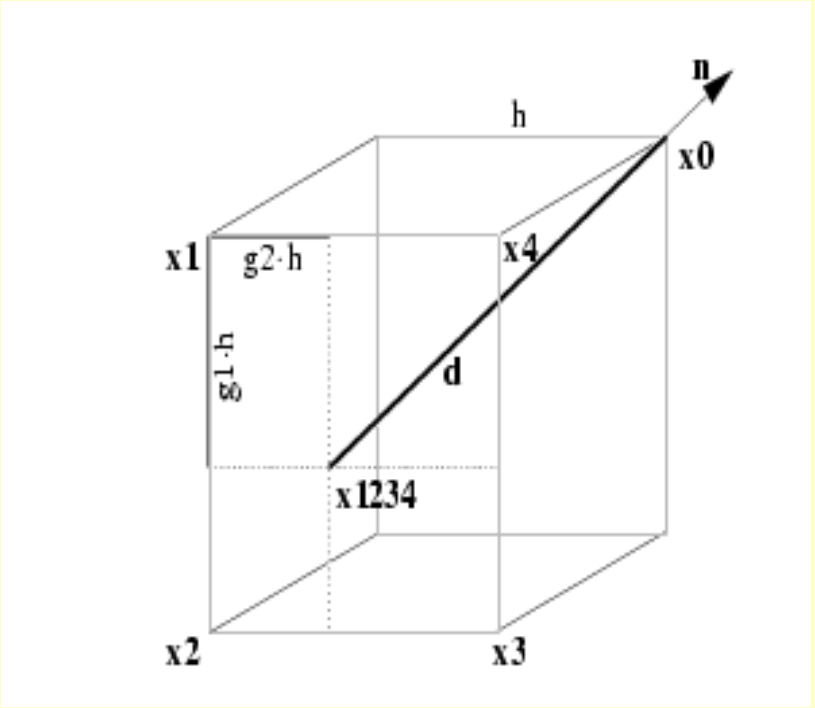
This inversion of T^m_h must not be done numerically!
(not fast enough, not accurate enough)

Suppose, T^m_h is lower triagonal. Then $T^m_h a = b$ has the solution:

$$a_i = b_i - \sum_{j=1}^{i-1} t_{ij} c_j \qquad (i = 1,...,n)$$

This is a direct, analytical formula to calculate
$(T^m_h)^{-1} b$ once T^m_h is known

1st order approximation to directional derivative $n_m \nabla_x I^m$:



$$n^m \nabla_x I^m(x_0) = I_0^m - \frac{I_{1234}^m}{d} + O(h)$$

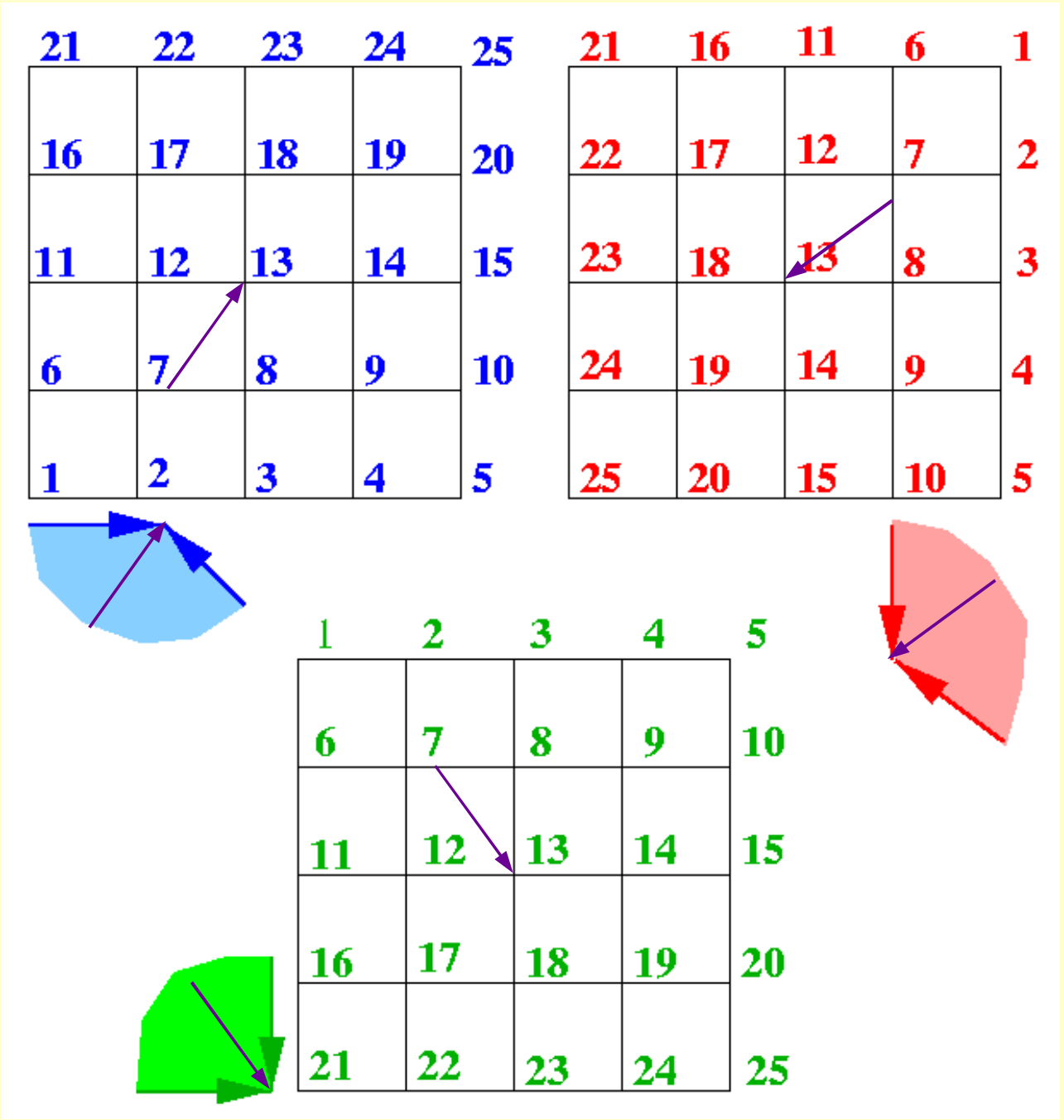
$$= I_0^m - I_1^m(1 - g_1 - g_2 + g_1 g_2) d^{-1} -$$
$$I_2^m(g_1 - g_1 g_2) d^{-1} - I_3^m(g_1 g_2) d^{-1} -$$
$$I_4^m(g_2 - g_1 g_2) d^{-1} + O(h)$$

Making T^m_{h-} lower triangular: Renumbering

(2D example)

Any given discrete ordinate direction m will fall into one of the three ranges of angel shown (blue, red, or green)

The numbering for each of these three ranges is such that the point the ordinate m is going to has always a higher number than any points limiting cell boundaries which have been crossed already by the ordinate.



$$T_h^m I_h^m = L_h \sum_{k=1}^{M} c^k I_h^k + \eta_h^m$$

$$\Leftrightarrow \quad I_h^m = (T_h^m)^{-1} L_h \sum_{k=1}^{M} c^k I_h^k + (T_h^m)^{-1} \eta_h^m$$

$$\Leftrightarrow \quad \underbrace{\sum_{m=1}^{M} c^m I_h^m}_{J_h} = \underbrace{\sum_{m=1}^{M} c^m (T_h^m)^{-1}}_{T_h} L_h \underbrace{\sum_{k=1}^{M} c^k I_h^k}_{J_h} + \underbrace{\sum_{m=1}^{M} c^m (T_h^m)^{-1} \eta_h^m}_{F_h}$$

$$\Leftrightarrow \quad J_h = T_h L_h J_h + F_h$$

$$\Leftrightarrow \quad (1_h - T_h L_h) J_h = F_h$$

Have now one system of equations for the mean intensity instead of one system per ordinate direction

The linear system $A_h J_h = E_h$

- A_h is definite for $\kappa \geq \lambda \geq 0$

– A_h is not symmetric

- A_h is a rather full matrix

- A_h is given only implicitly

At present, we solve $A_h J_h = F_h$ by a BiCGStab algorithm with diagonal preconditioning

(H.A. Van der Vorst, SIAM J. Sci. Stat. Comput., 1992, vol. 13, p. 631- 644)

Advantages:

- reduced h-dependence (due to $(T_h^m)^{-1}$)
- 'moderate' storage requirements
- fast convergence (in terms of BiCGStab iterations)

Problems:

- A_h is a full, non-symmetric matrix (few solvers work)
- κh has to be 'smaller' than 1 (fine discretization)
  convergence should deteriorate as
  $\lambda h \rightarrow \kappa h$ and $\kappa h \rightarrow 1$
- no error estimate as for finite element methods

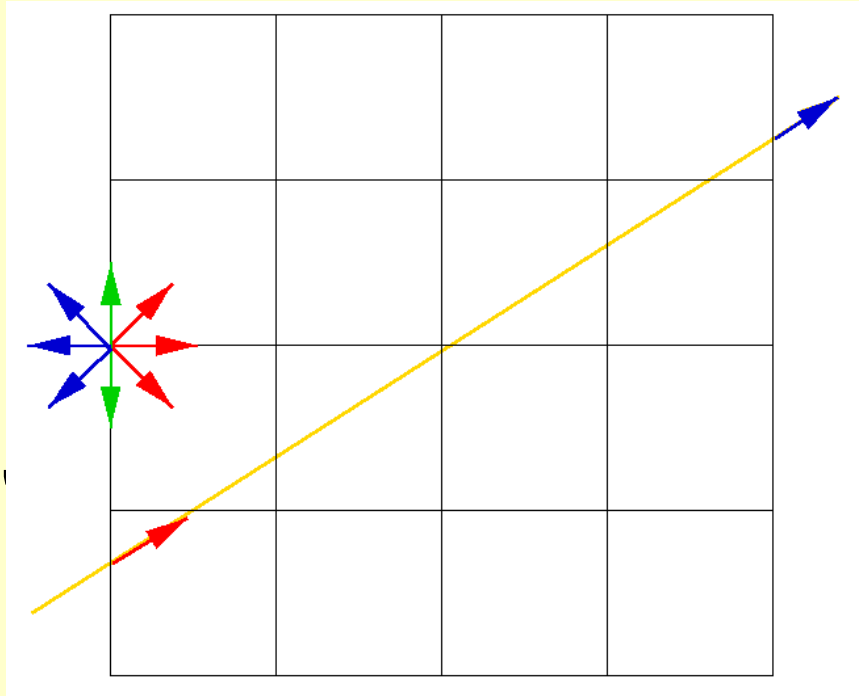
Boundary conditions

General situation:

Must specify boundary conditions at each boundary point of our spatial grid for each discrete ordinate direction m.

Have at each boundary point of our grid incoming as well as outgoing rays. There is no 'incomming boundary' as for hyperbolic problems.

Typically, a given discrete ordinate direction m is incoming on one side of the computational domain and outgoing on another side.

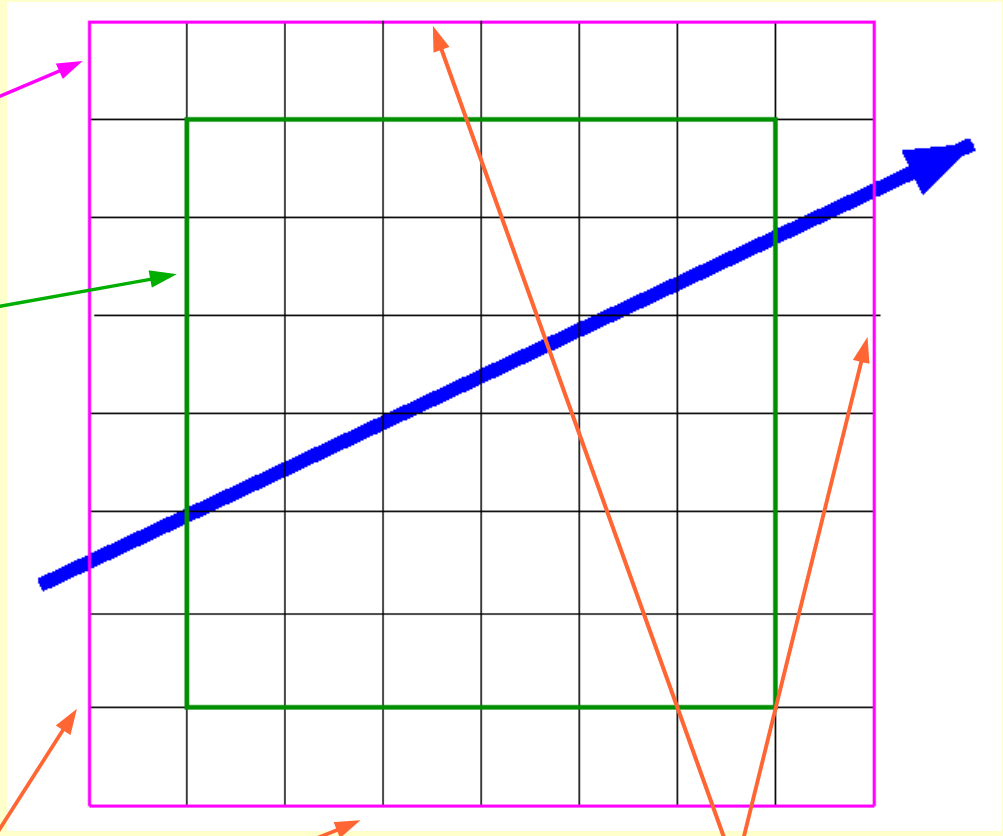


Open boundaries in TR3D

So far, we have used only open boundaries in TR3D

In practise, this means:

- add one layer of boundary cells around the computational grid
- solve for these additional cells the rate equations
- solve the transfer equation for outgoing directions
- set the specific intensiy I to some fixed value $\eta = f_{ext}$ you chose for incoming directions



set here $\eta = f_{ext}$; $\kappa = \lambda = 0$

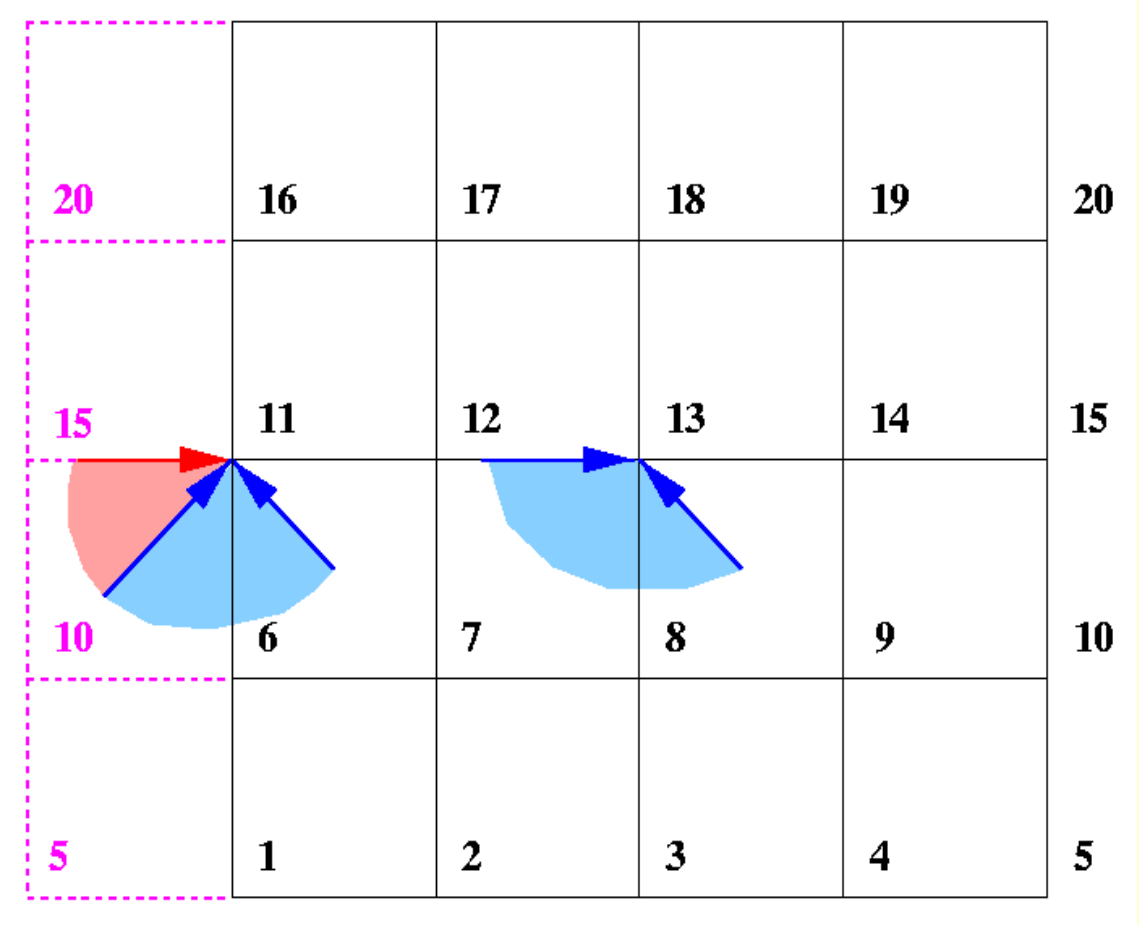
solve here the normal rate and transfer equations

Periodic boundaries: must iterate for boundary

black:
computaional grid
magenta:
virtual grid points for
periodic boundary

It is impossible to number the grid such that for the direction → point 15 has a lower number than point 15

⇒ For periodic boundaries the incoming specific intensity at point 11 at iteration step n must be taken as the outgoing intensity at point 15 at step n- 1



Adaptive mesh

Approach:

- cell by cell refinement
- refinement ratio 2
- mesh can be refined or coarsened
- optical depth as refinement criterion
- one mesh for all frequencies

Major new modules:

- definition of general data structure for point- by-point refined meshes
- efficient finding of next neighbours (must build T_h^m)
- numbering of mesh points (T_h^m triangular)

The rest of the code has not to be changed

Outlook

- possibility to have $I_1 = I_0\, e^{-d\tau}$ (instead of $I_1 = I_0\, [1-d\tau]$)

- (re-) parallelization
- further adaptivity:
  one mesh per frequency or per group of frequencies
  one mesh per ion or group of ions

- add more physics...

Numerical techniques in D3NEBEL

The transfer equation in D3NEBEL

D3NEBEL assumes nebular condition and an 'outward- only-approximation'. The transfer equation thus reduces to:

$$\underline{n} \cdot \nabla_x I^\nu = \eta^\nu - \underbrace{(\kappa^\nu + \lambda^\nu)}_{\chi} I^\nu$$

Along a single ray the equation is solved by:

$$J_\nu(r_{i+1}) = \left(\frac{r_i}{r_{i+1}}\right)^2 J_\nu(r_i) e^{-d\tau_\nu} + \frac{(r_{i+1}^3 - r_i^3)}{(3 r_{i+1}^2)} 4\pi e^{-d\tau_\nu} \sum_a \eta_a(\nu)$$

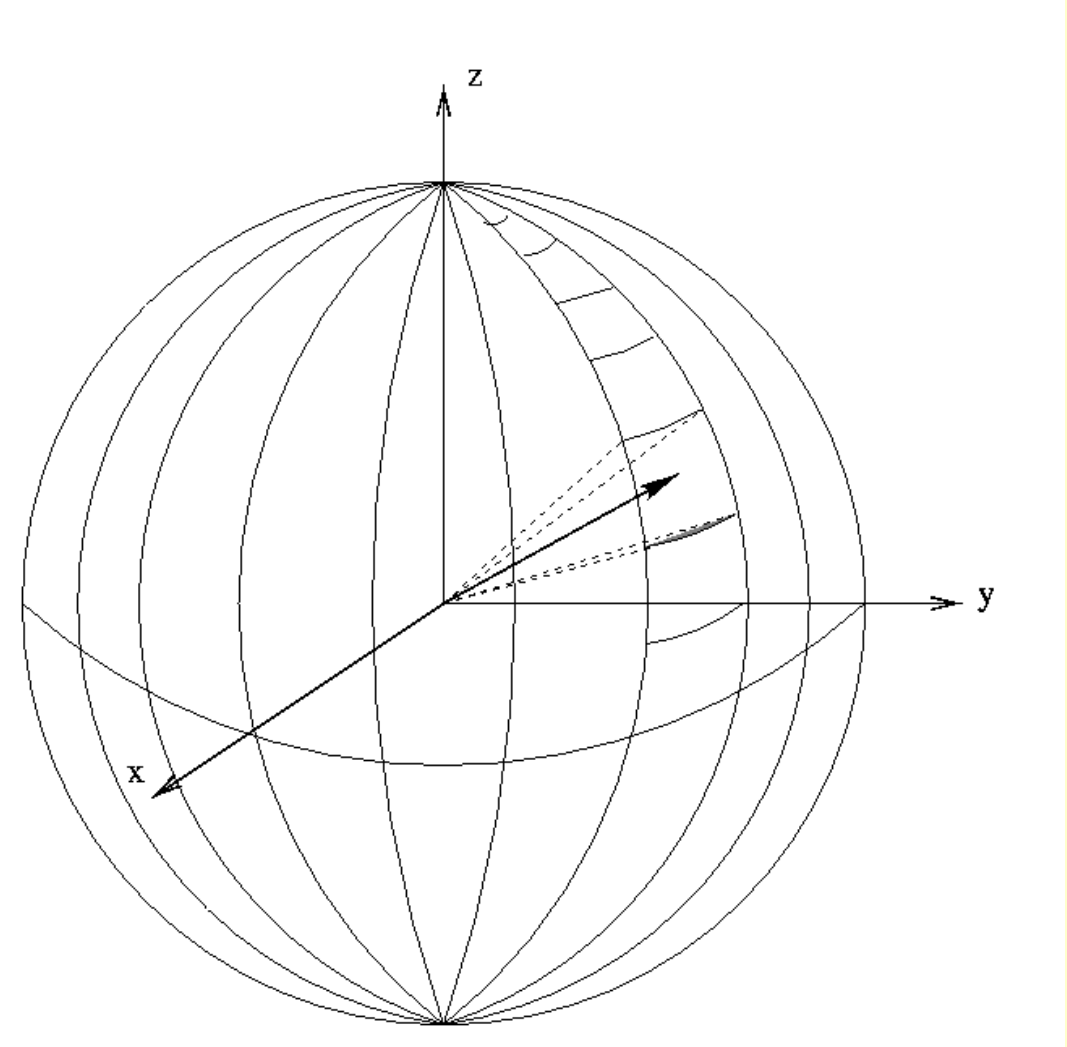
where the sum runs over all atomic emission processes considerd.

3D through a set of independent rays

Ordinate discretization analogous to that in TR3D.

However:
Now the individual discrete ordinates are completely independent from each other.

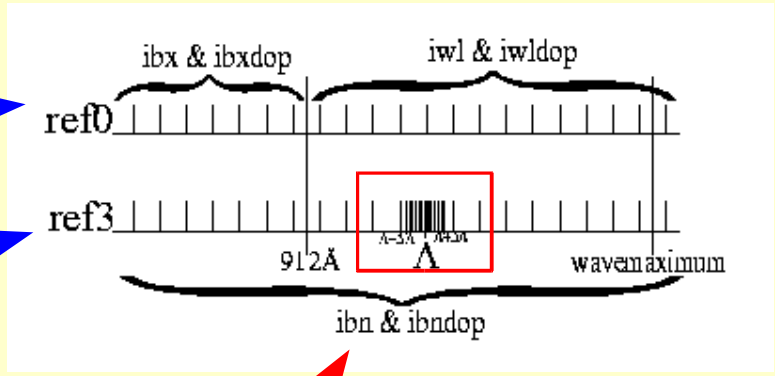
Only 'interaction' between individual ordinates:
Their contribution to the total spectrum is added up in the end.

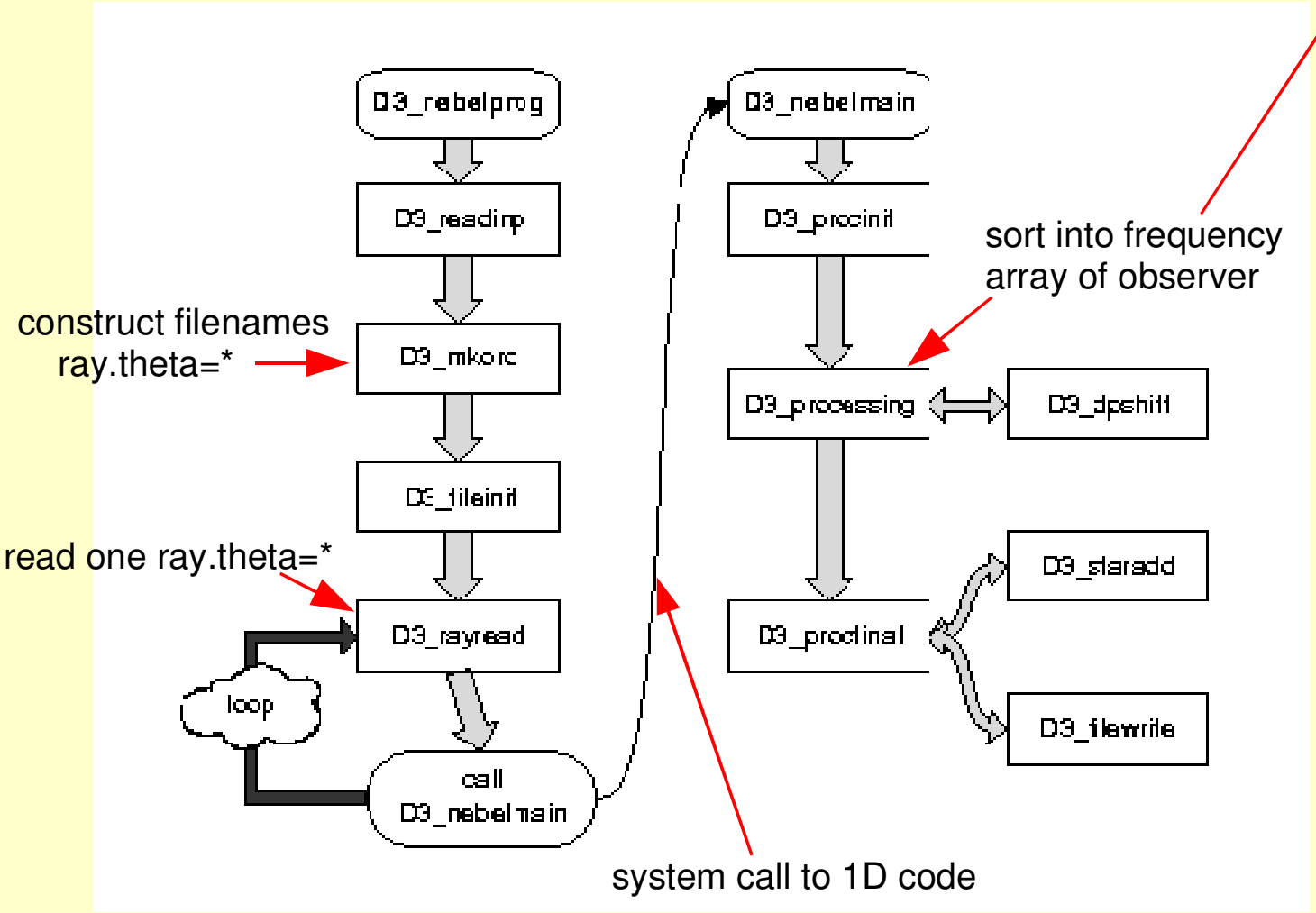


D3NEBEL schematically

frequency array for calculation along ray

frequency array for Doppler shifted spectrum, locally refined





Variable step size along one ray

0) start at radial distance r

1) make a step of size dr

2) iterate for ionization structure of H and He at r + dr
   no convergence within 10 steps $\Rightarrow$ dr $\rightarrow$ dr/2, goto 1)
   change in H or He too big with respect to r $\Rightarrow$ dr $\rightarrow$ dr/2, goto 1)

3) ionization structure of metals converged?
   no $\Rightarrow$ dr $\rightarrow$ dr/2, goto 1)

4) calculate new T_e
   no convergence $\Rightarrow$ dr $\rightarrow$ dr/2, goto 1)

5) accept step r $\rightarrow$ r + dr

Summary

TR3D: short characteristics, 1st order, discrete ordinates,
one equation for the mean intensities, BiGCStab solver,
3D (moderatly) thick NLTE radiative transfer

D3NEBEL: 3D through a set of 1D rays, adaptive spatial
step size along rays, nebular conditions