Numerical radiative transfer I

Contents

- The radiative transfer equation
- Limiting cases: diffusion and pure transport
- Different solution techniques: a survey
- Multidimensional radiative transfer
- Iterative solvers
- Summary

The radiative transfer equation

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

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

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

A Boltzmann equation for massless particles

Boltzmann equation is wide spread in physics

$\Rightarrow$ look also in other areas of physics and natural sciences for 'optimum' solution technique

neutron transport, atmospheric physics,
steel production (temperature of liquid steel),
biology (poisoning of bacteria)

(e.g. C. Cercignani, The Boltzmann equation and its applications, Springer, 1988

M. Pinar Mengüç, Radiative transfer I, Proceedings of the first international symposium on radiative transfer, Begell House, 1996

Diffusion limit

When $\chi^\nu \to \infty$ and $(\lambda^\nu / \chi^\nu) \to 1$ the radiative transfer equation

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

becomes (devide the equation by χ^ν and let $\chi^\nu \to \infty$ while $\lambda^\nu/\chi^\nu \to 1$)

$$I^\nu - \int_{S^2} d\Omega\, I^\nu = 0$$

In the diffusion limit, scattering dominates the problem.
Individual directions are 'thightly' coupled.

Any function which is angle- independent fullfills this equation

More precisely:
(Thesis of Klaus Jürgen Ressel, Colorado, 1994;
G.C. Pomraning, Diffusive limits for transport equations, Nuclear Science and Engineering 112, pp. 239- 255, 1992):

Let $\eta^\nu \to \varepsilon\eta^\nu$; $\chi^\nu \to 1/\varepsilon$; $\kappa^\nu \to \varepsilon$; and write $P\, I^\nu = \int_{S^2} d\,\Omega\, I^\nu$

Then the transfer equation can be rewritten as

$$\left[\underline{n} \cdot \nabla_x + \frac{1}{\epsilon}(1-P) + \epsilon\, P\right] I^\nu = \epsilon\, \eta^\nu$$

For $\varepsilon \to 0$ it can be shown that this equation goes to the diffiusion equation

$$-\nabla \cdot \left(\frac{1}{3\,\chi^\nu}\right) \nabla\, I^\nu + \kappa^\nu\, I^\nu = P\, \eta^\nu$$

The above scaling is particular in that the diffusion equation is independent of it.

Transport limit

When $\lambda^\nu \to 0$ the radiative transfer equation

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

becomes

$$\underline{n} \cdot \sum_x I^\nu = \eta^\nu - \kappa^\nu I^\nu$$

In the transport limit, individual directions are completely de- coupled.

The solution may be differnet for each angle

Contradictory demands of
the diffusion and the transport limit

Consequences for the numerical solution

The transfer equation in the transport limit is a hyperbolic problem.

$\Rightarrow$ need solver for hyperbolic PDE, need up-winding method

To obtain the correct behaviour of the numerical solution in the diffusion limit, the spatial discretization has to be such that

(Larsen, Morel, & Miller, JCP 83, 1989, p 212)

for a fixed mesh size h the discretization approximates a diffusion operator in the limit $\varepsilon \to 0$

Standard up- winding discretizations fail this condition

However, solutions exist

... at least for the case of neutron transport:

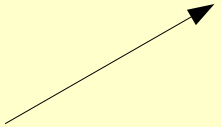
Larsen, Morel, & Miller, JCP 83, 1989, p 212
→ references to 'first attempts'

Manteuffel, Ressel, & Starke, SIAM J. Numer. Anal.
37/2, 2000,p 556
→ finite element discretization that wors for all regimes, from optically thick (diffusive) to optically thin (pure transport)

→ Manteuffel & Ressel, SIAM J. Numer. Anal. 35/2, 1997, p 806
reformulation of the transfer equation as just mentioned and frist solution approaches

Different solution techniques

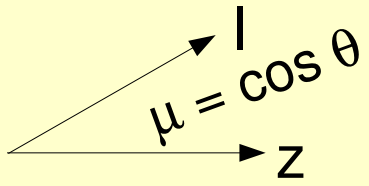
What transfer equation to solve?



Depending on physical system, transfer equation changes character

1D plane parallel, no scattering:
(ordinary differential equation)

$$\mu \frac{\partial I}{\partial z} = \eta - \chi I$$



1D plane parallel, with scattering:
(integro- differential equation)

$$\mu \frac{\partial I}{\partial z} = \eta - \chi I + \lambda \int_{S^2} d\Omega I$$

1D spherical, no scattering:
(partial differential equation)

$$\left[\mu \frac{\partial}{\partial r} + r^{-1}(1-\mu^2) \frac{\partial}{\partial \mu} \right] I = \eta - \chi I$$

THE solution technique does not exist

Plane parallel geometry: Feautrier

Write two equations governing incoming and outgoing radiation, $\pm\mu$

$$\pm\mu\left[\partial I(z\pm\mu,\nu)/\partial z\right]=\chi(z,\nu)\left[S(z,\nu)-I(z,\pm\mu,\nu)\right]$$

(S=source function = emission divided by losses)

Using $d\tau_\nu=d\tau(z,\nu)= -\chi(z,\nu)dz$ and $u(z,\mu,\nu) = \frac{1}{2}[I(z,\mu,\nu) + I(z,-\mu,\nu)]$
and $v(z,\mu,\nu) = \frac{1}{2}[I(z,\mu,\nu) - I(z,-\mu,\nu)]$ the above equation becomes

$$\mu^2\left[\partial^2 u_{\mu\nu}/\partial\tau_\nu^2\right]=u_{\mu\nu}-S_\nu$$

Have thus transformed transfer equation into a two- point boundary value problem (boundary values yet to be specified).
No particular closure needed.

Moment equations: widely used for 1D (2D, 3D)

Basic problem with radiativ transfer:
the solution for I depends on the zeroth order moment $J^\nu = \int_{S^2} d\,\Omega\, I^\nu$

$$\underline{n} \cdot \sum\nolimits_x I^\nu = \eta^\nu - \underbrace{\left(\kappa^\nu + \lambda^\nu\right)}_{\chi} I^\nu + \lambda^\nu J^\nu$$

Possible solution strategy:

Before solving transfer equation, solve its zeroth order moment $\rightarrow \mathrm{J}^\nu$

Before solving the zeroth oder moment, solve its first order moment $\rightarrow \mathrm{F}^\nu$

Before solving the zeroth oder moment, solve its first order moment $\rightarrow \mathrm{P}^\nu$

....

at some point, you have to terminate the series.

Possible closure relation: P^ν = function of J^ν

Monte Carlo techniques: especially for 3D

Basic idea:
send out N 'photon packets', one after the other, into a pre- defined density distribution (usually defined on a grid) and make a statistic of what happens to how many particles (get absorbed, shifted in wave- length, etc.)

Pros: simple to code, can handle any geometry

Cons: expensive, if high accuracy is desired or if dimensionality is small (<6 to 10)

Multidimensional radiative transfer

Essentially three approaches

Monte Carlo techniques:

wide spread, easy to code, flexible with regard to geometry, but expensive for small dimensions or high accuracy

Long characteristics:

usually too expensive, but may be usefull for applications where high accuracy is desired and the transport limit is reached (at least in part of the domain)

Short characteristics:

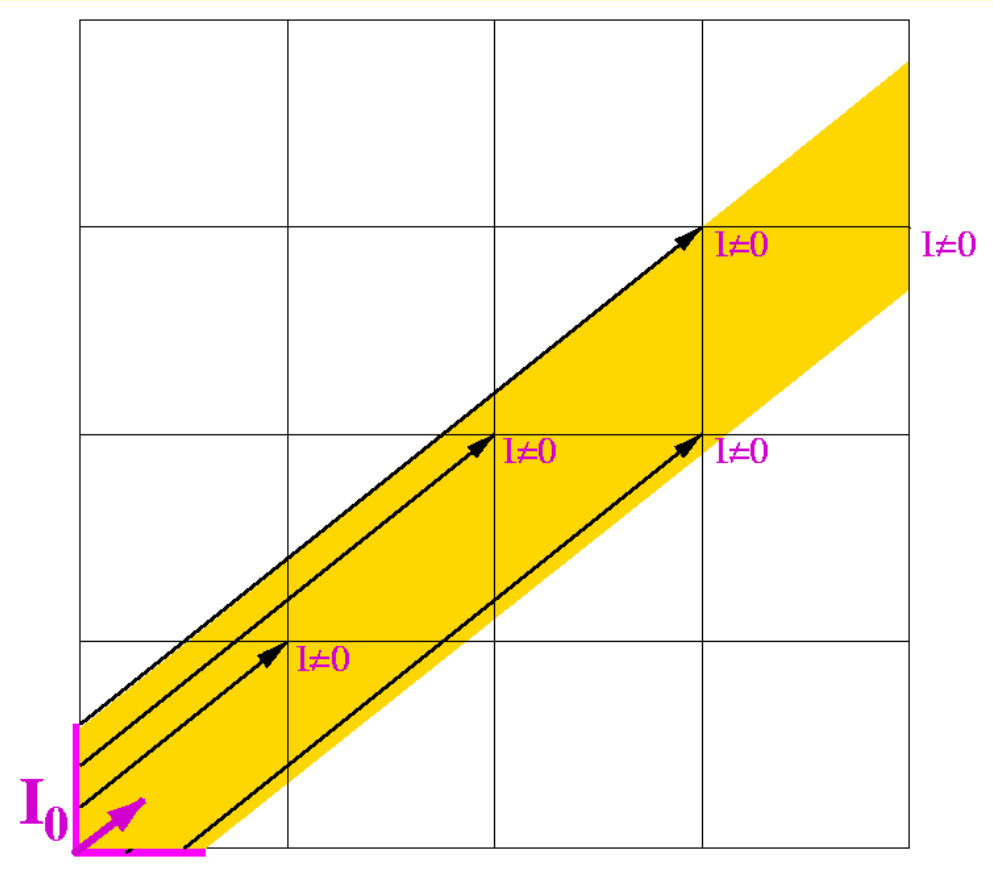
wide spread, not statistical thus 'more controlable', difficult to code, must solve large linear systems of equations

Long characteristics

From each grid point, go back in the direction of the currently handled discrete ordinate m.

If you hit the source, compute transfer along this ray from the source to current grid point. 'On the way', use data on grid.

Problem:
for each ordinate direction m, and for a substantial fraction of the total number of grid points you have, you need to compute a ray of length 'about the size of the computational domain'
⇒ very expensive



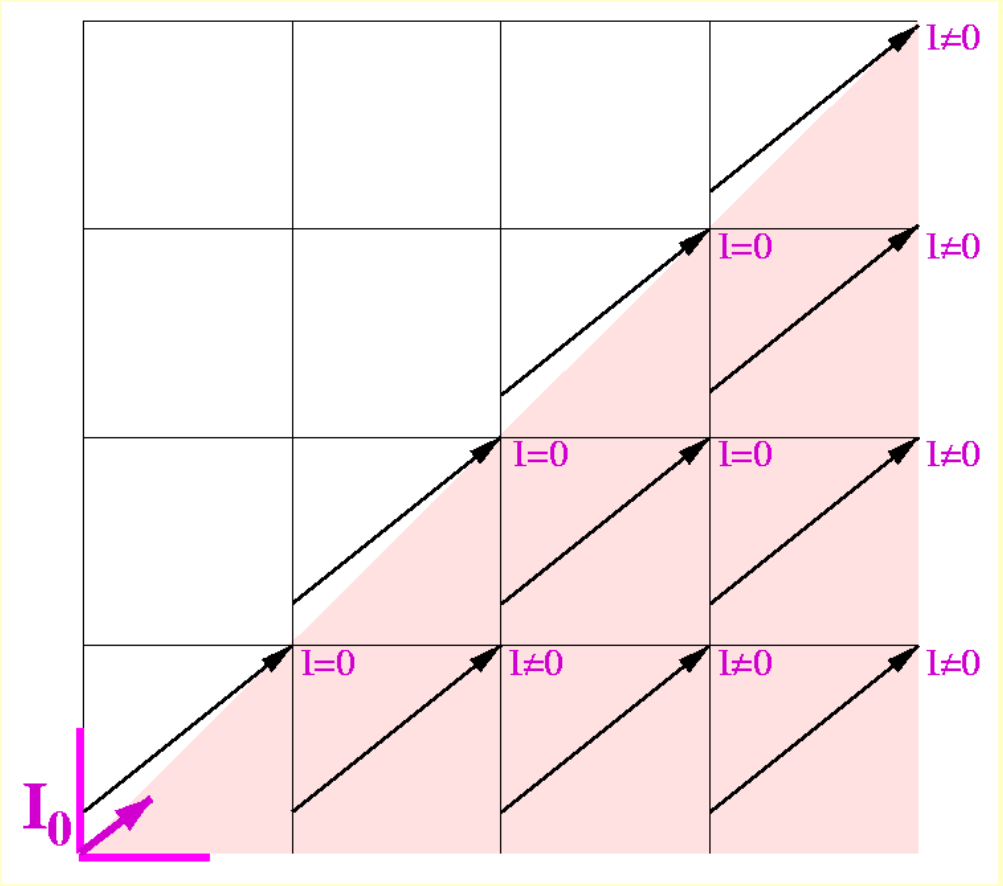
Short characteristics

For a given ordinate direction, for each grid point, go back in the direction of the ordinate until you hit the first cell boundary.

Interpolate needed quantities at this intersection point from grid values.

Solve the transfer equation from the intersection point to the current grid point.

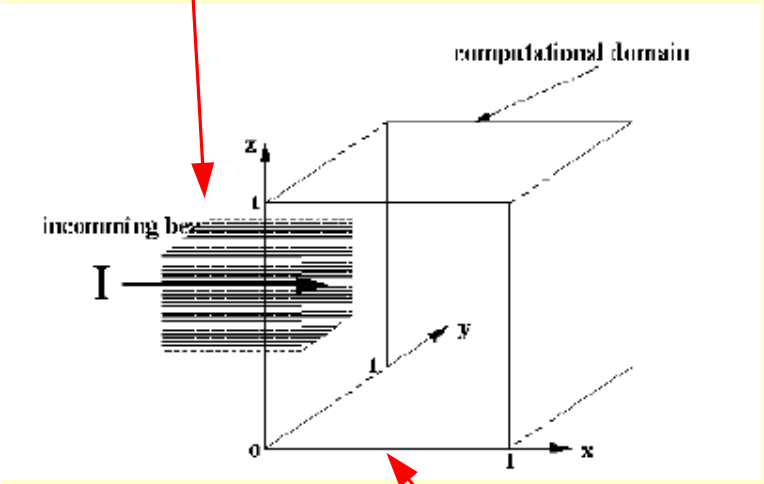
Problem: Beam widening.



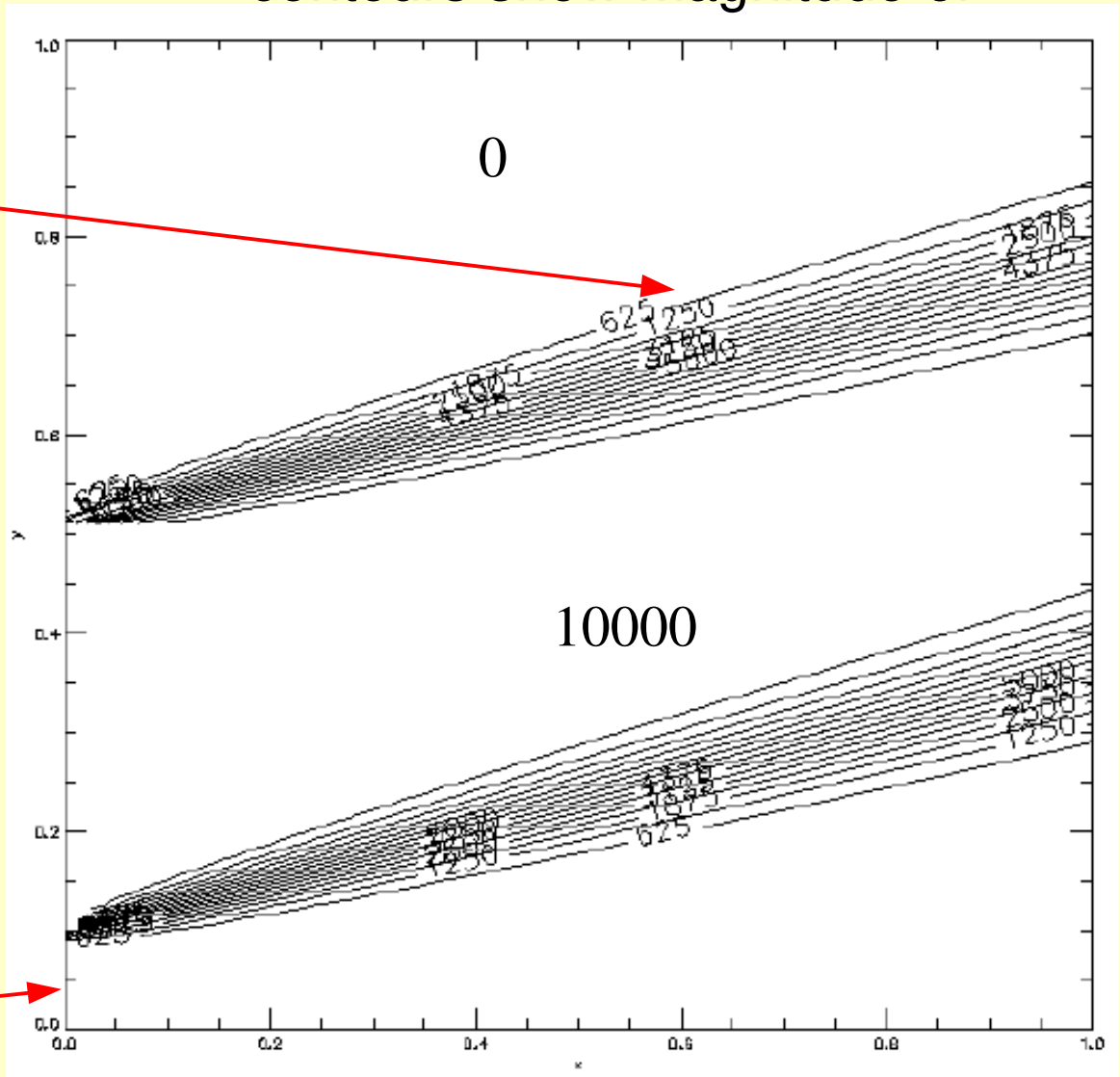
Beam widening with short characteristics

contours show magnitude of I

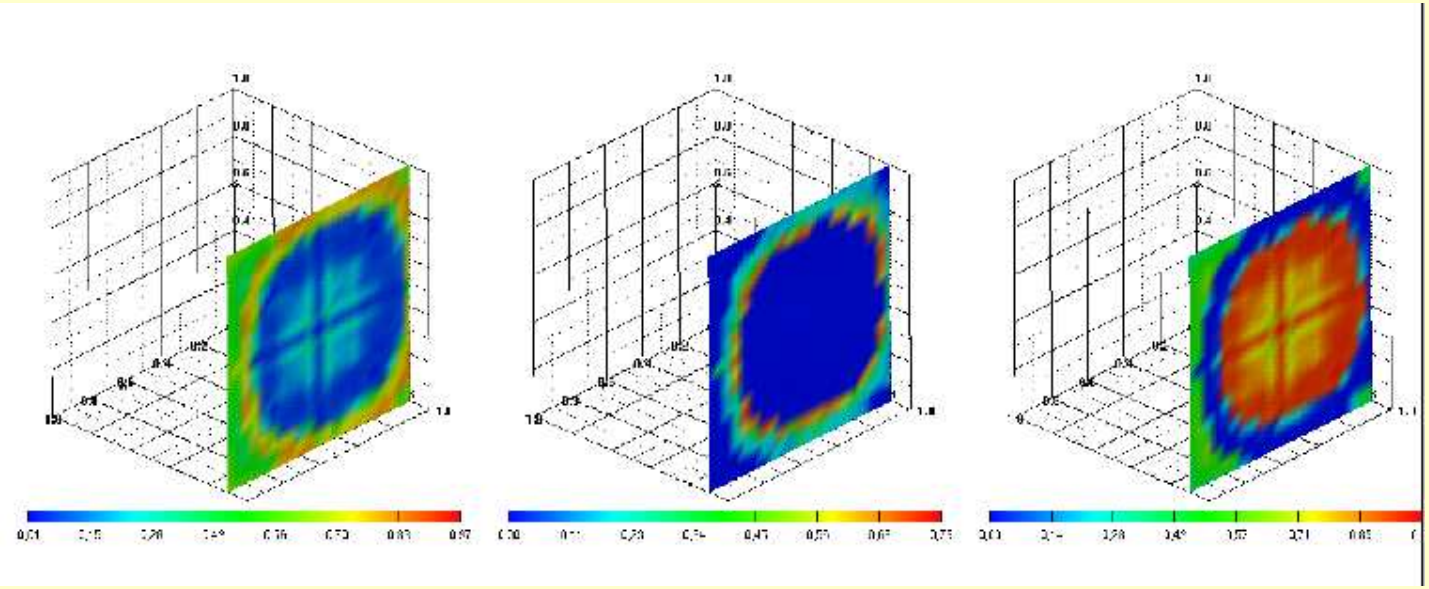
directed beam
of radiation

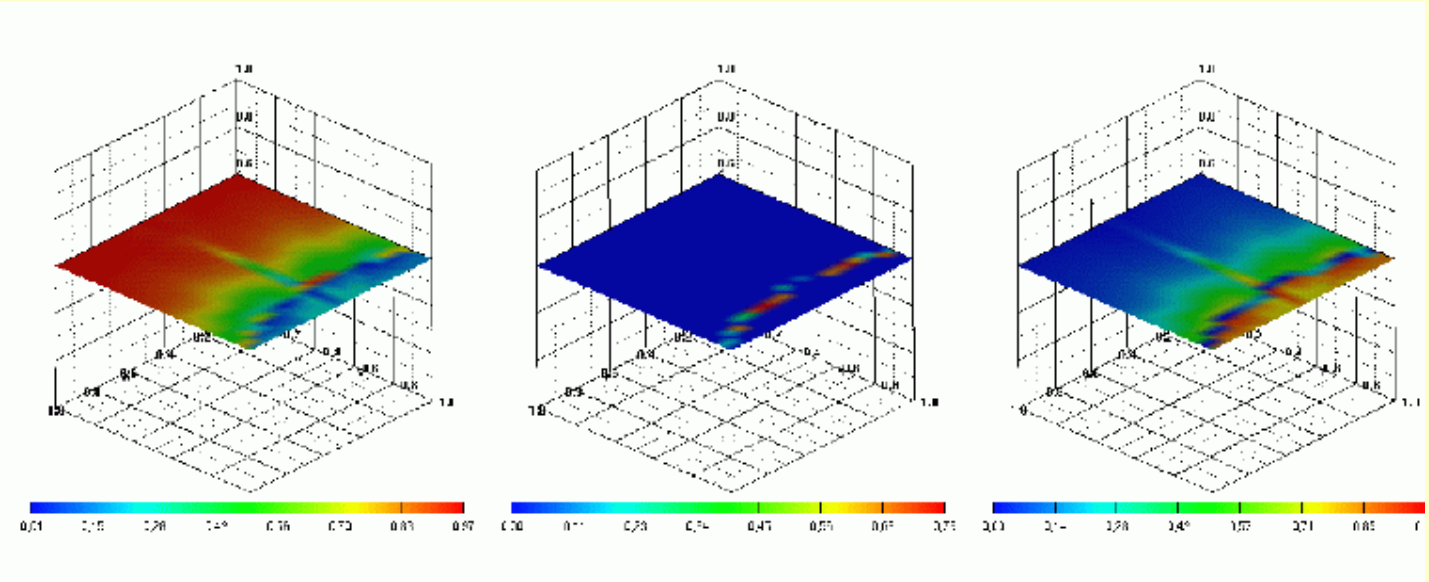


Computational
domain



Alignement effects with short characteristics





Solving linear systems of equations

Linear systems of equations: direct solutions

Direct solution $\Leftrightarrow$ given $Ax=b$ you calculate $x_i = f(A,b,x_j)$
where x_i are the components of x and $j < i$

Advantage: There is the one solution
Difficulty: For large systems, numerical errors accumulate.
Number of operations too time consuming ($O(n^3)$)

For small system (< 1000 unknowns) direct solutions
are often best, but take the right method!

Generally: 1) $A = ST$; 2) $Sc - b = 0$; 3) $Tx + c = 0$;

LR factorization (Gauss): $A = LR$

Decomposition into L and R usually deteriorates condition number of the system, thus the accuracy of the solution.
Pivoting usually a must, but can be difficult.
Works for non- singular n x n- systems.

QR factorization (Housholder / Givens): $A = QR$

QR decomposition preserves the condition number of the system.
Housholder encounters problems when columns of A are nearly linearly dependent.
Works for general n x m - systems.

Cholesky: $A = LL^T$ or $A = R^TR$

Preserves condition number of the system.

Works only for symetric positive- definite n x n systems.

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software on the web:
http:// www.netlib.org/lapack
background on the web:
http:// www.psc.edu/~burkardt/papers/linear_glossary.html

Linear systems of equations: iterative solutions

Iterative solution $\Leftrightarrow$ given $Ax=b$ you calculate $x_n = f(A,b,x_m)$
where x_n are successive approximations
to the solution x and $m < n$

Advantage: simple (only matrix - vector multiplications)
Difficulty: The x_n may approach the solution x only slowly or not at all.
You get only an approximation x_n to the solution x
$\Rightarrow$ must decide when you are 'close enough to x'

For large non- banded linear systems (n>10'000) iterative solution methods are usually best!

A) stationary iterative methods or splitting techniques:

1) splitt $A = C + R$

2) solve $Cx_{l+1} = - Rx_l + b$ for x_{l+1} [formally: $x_{l+1} = C^{-1}(- Rx_l + b)$]

Tradeoff necessary: i) C^{-1} should be 'nearly' A^{-1} $\Rightarrow$ $C = A$

ii) $Cx_{l+1} = - Rx_l + b$ easy to solve $\Rightarrow$ $C = \mathrm{diag}(A)$

Examples:

Jaccobi: $A = E + D + F$; $Dx_{l+1} = - (E + F)x_l + b$

(use only components of x_l to compute x_{l+1}; slow convergence)

Gauss- Seidel: $A = E + D + F$; $(D+E)x_{l+1} = - Fx_l + b$

(to compute component m of x_{l+1} use components i=1,..,m- 1 of x_{l+1} and components i= m,..,n of x_l ; sligthly faster convergence than Jaccobi)

SOR: $A = E + D + F$; $(1/\omega\, D+E)x_{l+1} = (- F+(1/\omega - 1)D)x_l + b$

(Gauss- Seidel but with weight- function ω. Depending on choice of ω, convergence is faster (1 order of magnitude) or slower than for Gauss- Seidel)

B) non- stationary iterative methods (minimum residuum, conjugate gradient, Lanczos-type, Krylov sub- space)

Basic idea: minimize the residual functional $f(x) = (Ax - b)^T(Ax - b)$
over a sequence of vector spaces $V_k = \{r_0, Ar_0, ..., A^k r_0\}$
(V_k =Krylov sub- space; $r_0 = Ax_0$; x_0 = starting vector).
At each iteration step, V_k is enlarged by 1dimension.
After n steps, V_n spans the whole space and $f(x) = 0$.

Two 'flavours':

1) use V_k only implicitly; compute x_k and r_k based on only the last two or three x_k and r_k
2) use V_k only explicitly; compute x_k and r_k based on only the last two or three x_k and r_k but then explicitly minimize r_k over V_k

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2) is much more costly than 1)

- have to store entire vector space V_k (= k vectors of length n)
- have to explicitly minimize a vector with regard to V_k

Two 'flavours':

1) use V_k only implicitly; compute x_k and r_k based on only the last two or three x_k and r_k

2) use V_k only explicitly; compute x_k and r_k based on only the last two or three x_k and r_k but then explicitly minimize r_k over V_k

- If A is symmetric and positive definite, 1) will give the same as 2)

- If A is not symmetric and positive definite, 2) will smoothly converge, 1) will converge non- monotonically or not at all

- Preconditioning is essential for 1) and 2): $Ax=b \rightarrow PAx = b$

- 2) may be 'restarted': After m steps, throw away part of V_k and continue with the rest. Convergence becomes spurious again.

Examples for 1): CG; CGS; BiCG; BiCGStab; BiCGStab(l)

Examples for 2): CGR; MINRES; GMRES; GMRES(m); (FOM);

Literature

http:// www.netlib.org/linalg/old_html_templates/chapter2.6.html

http:// www.sam.math.ethz.ch/~mhg

http:// www.cs.utk.edu/~dongarra/etemplates/node390.html

http:// www.mcc.uiuc.edu/SummerSchool/Eric%20de%20Sturler/desturler.html

Axelsson, Iterative Solution Methods, Cambridge University Press

Kelley, Iterative Methods for Linear and Nonlinear Equations,
Frontiers in Applied Mathematics, SIAM

Summary

- Radiative transfer equation is a Boltzmann equation.
  There exists extensive literature on numerical solution of the later.

- The diffusion limit and the transport limit of the radiative transfer equation are 'in contradiction' with regard to the numerical method

- How to solve the transfer equation depends on what physical problem you look at (dimensionality, scattering)

- For multi- dimensional radiative transfer Monte Carlo techniques and short characteristics today are methods of choice.
  Both have their merits and draw- backs.

- Iterative solvers: direct methods vs. iterative methods,
  take a moment to make the right choice