Mathematical modelling for dose deposition in photontherapy

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PhD defense
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Work realized under the supervision of:

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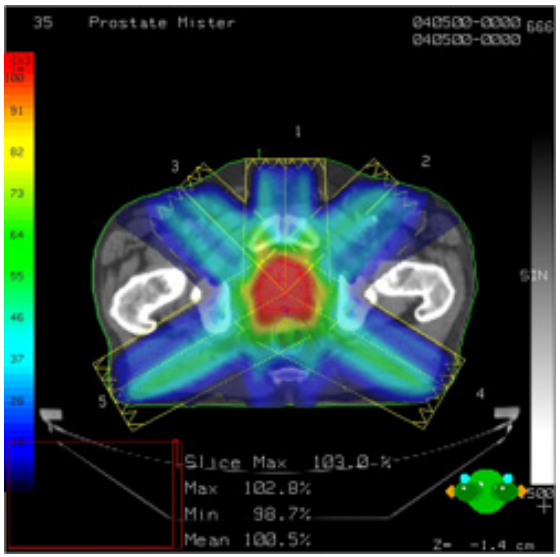
Context

In 2012: **14.1 million** cancers diagnosed around the world

Types of treatements: radiotherapy, surgery and chemotherapy

$$\text{Radiations} \equiv \text{beams of particles}$$

$$\text{Deposited energy (dose)} \Rightarrow \text{Biological effects}$$



Objectives:

Dose computation **fast** and **accurate**

$\hookrightarrow$ Optimization algorithm

Available models

Transport of particles:

- **Kinetic level**
  $\hookrightarrow$ numerically too costly (Monte Carlo, DOM)
- **Angular moment approach**
  $\hookrightarrow$ good compromise
- **Hydrodynamic level**
  $\hookrightarrow$ unsufficient for the present medical applications

Present work

Kinetic model:

- Modelling
- Conservation properties
- Well-posedness

Moment model:

- Modelling
- Domain of validity
- Computation of closures

Numerical schemes:

- Non-linear equations
- Fast characteristics problem

Optimization algorithm:

- Projected gradient algorithm

Main difficulties:

- Numerical computations of moment closures
- Time-efficient schemes in low density media

Kinetic equations

Fluence

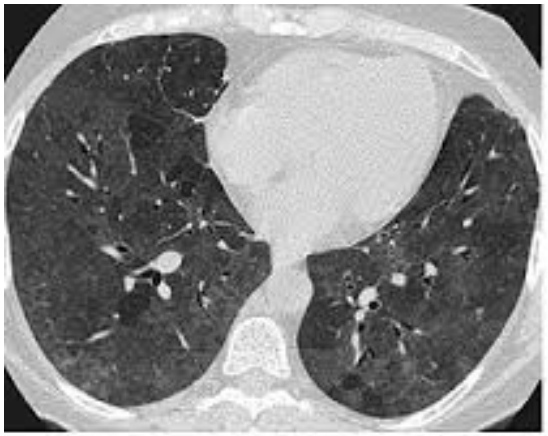
$$dN = \psi(\epsilon, x, \Omega) d\epsilon dx d\Omega \quad \geq \quad 0$$

Energy $\epsilon \in [\epsilon_{\min}, \epsilon_{\max}]$, Position $x \in Z$, Direction of flight $\Omega \in S^2$

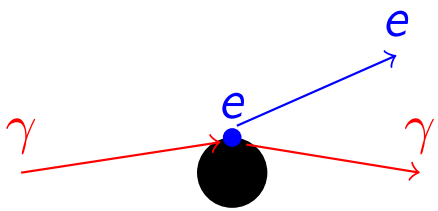
Kinetic equations

$$\begin{aligned} \Omega.\nabla_x \psi_\gamma &= \rho \left(Q_{\gamma\to\gamma}(\psi_\gamma) + Q_{e\to\gamma}(\psi_e) \right), \\ \Omega.\nabla_x \psi_e &= \rho \left(Q_{e\to e}(\psi_e) + Q_{\gamma\to e}(\psi_\gamma) \right), \end{aligned}$$

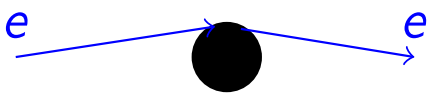
Relative density $\rho \in [10^{-3}, 2]$



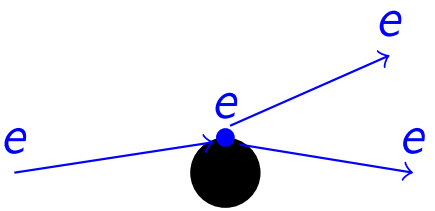
Kinetic equations



Compton collision



Mott collision



Møller collision

Collision operators

$$
\begin{aligned}
Q_{\gamma\to\gamma}(\psi_\gamma) &= \overbrace{}^{\text{CSDA}^1} + \overbrace{G_{\gamma\to\gamma}(\psi_\gamma)}^{\text{LB gain}} - \overbrace{P_\gamma(\psi_\gamma)}^{\text{LB loss}},\\
Q_{e\to e}(\psi_e) &= \partial_\epsilon(S\psi_e) + G_{e\to e}(\psi_e) - P_e(\psi_e),\\
Q_{\gamma\to e}(\psi_\gamma) &= G_{\gamma\to e}(\psi_\gamma),\\
Q_{e\to\gamma}(\psi_e) &= 0,
\end{aligned}
$$

for $\alpha, \beta = \gamma, e$,

$$P_\alpha(\psi_\alpha)(\epsilon, x, \Omega) = \sigma_{T,\alpha}(\epsilon)\psi_\alpha(\epsilon, x, \Omega),$$

$$G_{\alpha\to\beta}(\psi_\alpha)(\epsilon, x, \Omega) = \int_\epsilon^{\epsilon_{\max}} \int_{S^2} \sigma_{\alpha\to\beta}(\epsilon', \epsilon, \Omega'.\Omega)\psi_\alpha(\epsilon', x, \Omega')d\Omega' d\epsilon',$$

$\hookrightarrow$ solved backward in ϵ

$\hookrightarrow$ $\epsilon \equiv$ numerical time

[1] Pomraning, *Math. Mod. Meth. Appl. S.*, 1992

Kinetic model

Kinetic equations

$$\begin{aligned}
\Omega.\nabla_x \psi_\gamma &= \rho \qquad\qquad (G_{\gamma\to\gamma} - P_\gamma)(\psi_\gamma), \\
\underbrace{\Omega.\nabla_x \psi_e}_{\text{transport}} &= \rho\Big[\underbrace{\partial_\epsilon(S\psi_e)}_{\text{CSDA}} + \underbrace{(G_{e\to e} - P_e)(\psi_e)}_{\text{linear Boltzmann}} + \underbrace{G_{\gamma\to e}(\psi_\gamma)}_{\text{coupling}}\Big],
\end{aligned}$$

Dose: energy transfered per mass unit

$$D(x) = \int_{\epsilon_{min}}^{\epsilon_{max}} \int_{S^2} \epsilon \left[Q_{\gamma\to\gamma}(\psi_\gamma) + Q_{\gamma\to e}(\psi_\gamma) + Q_{e\to e}(\psi_e)\right](\epsilon, x, \Omega) d\Omega d\epsilon$$

Moments

Aim: reduce computation costs

Moment methods:

$$\begin{array}{ccc} \text{Kinetic} & & \text{Moments} \\ \psi(\epsilon, x, \Omega) & \leftrightarrow & \boldsymbol{\psi}(\epsilon, x) \end{array}$$

$$\textbf{Tensorial notation} \quad \psi^i(\epsilon, x) = \int_{\Omega \in S^2} \underbrace{\Omega \otimes \cdots \otimes \Omega}_{\text{i times}} \psi(\epsilon, x, \Omega) d\Omega,$$

$$\begin{array}{ccc} \psi^0 & \rightarrow & \text{density} \\ \psi^1 & \rightarrow & \text{flux} \\ \psi^2 & \rightarrow & \text{pressure} \end{array}$$

$$\textbf{Vectorial notation} \quad \boldsymbol{\psi}(\epsilon, x) = \int_{\Omega \in S^2} \mathbf{m}(\Omega) \psi(\epsilon, x, \Omega) d\Omega,$$

First order equations

Orders 0 and 1

$$\gamma \quad \begin{cases} \nabla_x.\psi_\gamma^1 = & \rho(G_{\gamma\to\gamma}^0 - P_\gamma^0)(\psi_\gamma^0) \\ \nabla_x.\psi_\gamma^2 = & \rho(G_{\gamma\to\gamma}^1 - P_\gamma^1)(\psi_\gamma^1) \end{cases}$$

$$e\_ \quad \begin{cases} \nabla_x.\psi_e^1 = & \rho\left[\partial_\epsilon(S\psi_e^0) + (G_{e\to e}^0 - P_e^0)(\psi_e^0) + G_{\gamma\to e}^0(\psi_\gamma^0)\right] \\ \nabla_x.\psi_e^2 = & \rho\left[\partial_\epsilon(S\psi_e^1) + (G_{e\to e}^1 - P_e^1)(\psi_e^1) + G_{\gamma\to e}^1(\psi_\gamma^1)\right] \end{cases}$$

$\hookrightarrow$ **requires a closure**

$$\psi_\gamma^2 = f_\gamma(\psi_\gamma^0, \psi_\gamma^1), \quad \psi_e^2 = f_e(\psi_e^0, \psi_e^1)$$

Second order model

Order 2

$$\begin{array}{cl} \gamma & \left\{ \nabla_x . \psi^3_\gamma = \rho(G^2_{\gamma\to\gamma} - P^2_\gamma)(\psi^2_\gamma) \right. \\ e & \left\{ \nabla_x . \psi^3_e = \rho\left[\partial_\epsilon(S\psi^2_e) + (G^2_{e\to e} - P^2_e)(\psi^2_e) + (G^2_{\gamma\to e})(\psi^2_\gamma)\right] \right. \end{array}$$

$\hookrightarrow$ **requires a closure**

$$\psi^3_\gamma = g_\gamma(\psi^1_\gamma, \psi^2_\gamma), \quad \psi^3_e = g_e(\psi^1_e, \psi^2_e)$$

General notation

Rewritten equation

$$\nabla_x . F = \rho \mathbf{Q}(\boldsymbol{\psi}),$$

$$\begin{aligned}
\boldsymbol{\psi} &= (\boldsymbol{\psi}_\gamma,\ \boldsymbol{\psi}_e), \qquad F = (F_\gamma,\ F_e), \\
\mathbf{Q}(\boldsymbol{\psi}) &= \left((\mathbf{G}_{\gamma\to\gamma} - \mathbf{P}_\gamma)(\boldsymbol{\psi}_\gamma),\quad \partial_\epsilon(S\boldsymbol{\psi}_e) + (\mathbf{G}_{e\to e} - \mathbf{P}_e)(\boldsymbol{\psi}_e) + \mathbf{G}_{\gamma\to e}(\boldsymbol{\psi}_\gamma) \right),
\end{aligned}$$

$$\begin{aligned}
\text{for} \quad \alpha &= \gamma, e \\
\boldsymbol{\psi}_\alpha &\equiv \int_{S^2} \mathbf{m}(\Omega)\psi_\alpha(\Omega)d\Omega, \qquad F_\alpha \equiv \int_{S^2} \Omega \otimes \mathbf{m}(\Omega)\psi_\alpha(\Omega)d\Omega
\end{aligned}$$

$\hookrightarrow$ **requires a closure** $\qquad F_\gamma(\boldsymbol{\psi}_\gamma) \qquad F_e(\boldsymbol{\psi}_e)$

Common construction of the closure

Moments

ψ

Common construction of the closure

$$\text{Moments} \quad \rightarrow \quad \text{Ansatz}$$

$$\boldsymbol{\psi} \quad \rightarrow \quad \psi_R(\Omega)$$

Ansatz ψ_R in

$$\mathcal{C}(\boldsymbol{\psi}) \quad = \quad \left\{ \psi \quad , \quad \int_{S^2} \mathbf{m}(\Omega)\psi(\Omega)d\Omega = \boldsymbol{\psi} \right\} \quad ,$$

Common construction of the closure

$$\text{Moments} \quad \rightarrow \quad \text{Ansatz} \quad \rightarrow \quad \text{Closure}$$

$$\boldsymbol{\psi} \quad \rightarrow \quad \psi_R(\Omega) \quad \rightarrow \quad F \approx \int_{S^2} \Omega \otimes \mathbf{m}(\Omega)\psi_R(\Omega)d\Omega$$

Ansatz ψ_R in

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$$\mathcal{C}(\boldsymbol{\psi}) \quad = \quad \left\{ \psi \geq 0, \quad \int_{S^2} \mathbf{m}(\Omega)\psi(\Omega)d\Omega = \boldsymbol{\psi} \right\} \quad ,$$

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Realizability domain

$$\mathcal{R}_{\mathbf{m}} \quad = \quad \left\{ \boldsymbol{\psi} \in \mathbb{R}^{Card(\mathbf{m})}, \quad \text{s.t.} \right.$$

$$\left. \exists \psi \in L^1(S^2), \quad \psi \geq 0, \quad \boldsymbol{\psi} = \int_{S^2} \mathbf{m}(\Omega)\psi(\Omega)d\Omega \right\}$$

Properties of the realizability domain

Proposition

$\mathcal{R}_{\mathbf{m}}$ is an open convex cone

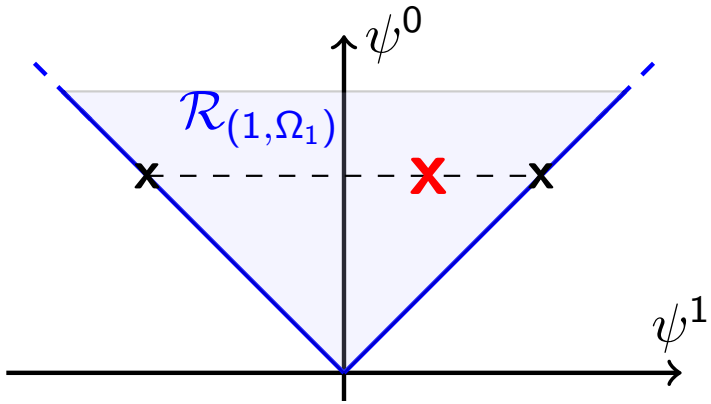
$$\forall \quad \alpha_1 > 0,\ \alpha_2 > 0, \quad \boldsymbol{\psi}_1 \in \mathcal{R}_{\mathbf{m}},\ \boldsymbol{\psi}_2 \in \mathcal{R}_{\mathbf{m}}, \qquad \alpha_1\boldsymbol{\psi}_1 + \alpha_2\boldsymbol{\psi}_2 \in \mathcal{R}_{\mathbf{m}}$$

$\hookrightarrow$ construction of numerical schemes

Proposition

If $\boldsymbol{\psi} \in \partial\mathcal{R}_{\mathbf{m}}$, then there exists a measure γ s.t.

$$\boldsymbol{\psi} = \int_{S^2} \mathbf{m}(\Omega) d\gamma(\Omega)$$



$\hookrightarrow$ computation of the closure

Characterization of the realizability domain[2,3]

Proposition (First order moments)

Choose $\mathbf{m}(\Omega) = (1, \Omega)$, *then*

$$\mathcal{R}_{\mathbf{m}} = \left\{ \boldsymbol{\psi} \in \mathbb{R}^4, \quad s.t. \quad |\psi^1| < \psi^0 \right\} \cup \{0_{\mathbb{R}^4}\}$$

If $\quad |\psi^1| = \psi^0, \quad$ *then* $\quad \gamma = \psi^0 \delta\left(\Omega - \frac{\psi^1}{\psi^0}\right)$

Proposition (Second order moments)

Choose $\mathbf{m}(\Omega) = (\Omega_1,\ \Omega_2,\ \Omega_3,\ \Omega_1^2,\ \Omega_2^2,\ \Omega_3^2,\ \Omega_1\Omega_2,\ \Omega_1\Omega_3,\ \Omega_2\Omega_3)$, *then*

$$\mathcal{R}_{\mathbf{m}} = \left\{ \boldsymbol{\psi} \in \mathbb{R}^9, \quad s.t. \quad |\psi^1| < tr(\psi^2), \right.$$
$$\left. tr(\psi^2)\psi^2 - \psi^1 \otimes \psi^1 > 0 \right\} \cup \{0_{\mathbb{R}^9}\}$$

[2] Kershaw, 1976
[3] Akhiezer, 1962

M_1 closure

$$\text{Moments} \quad \rightarrow \quad \text{Ansatz} \quad \rightarrow \quad \text{Closure}$$

$$(\psi^0, \psi^1) \quad \rightarrow \quad \psi_{M_1}(\Omega) \quad \rightarrow \quad \psi^2 \approx \int_{S^2} \Omega \otimes \Omega \psi_{M_1}(\Omega) d\Omega$$

Ansatz ψ_{M_1} in

$$\mathcal{C}_1 \quad = \quad \left\{ \psi \geq 0, \quad \int_{S^2} \psi d\Omega = \psi^0, \quad \int_{S^2} \Omega \psi d\Omega = \psi^1 \right\} \neq \emptyset \text{ if } \quad \boldsymbol{\psi} \in \mathcal{R}_{\mathbf{m}},$$

Choice of the ansatz[4,5]

$$\psi_{M_1} = \underset{\psi \in \mathcal{C}_1}{\operatorname{argmin}}(\mathcal{H}(\psi)) \quad \Rightarrow \quad \psi_{M_1} = \exp(S + V.\Omega),$$

[4] Minerbo, *J. Quant. Spect. Rad. Transfer*, 1977
[5] Levermore, *J. Stat. Phys.*, 1995

M_1 closure

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Advantages:

- Symmetric hyperbolic[5]
- Realizable
- Entropy decay[5]
- Accurately models beams

Numerical cost:

- minimization problem
- numerical quadrature

Alternative computation:

$$\psi^2 = \psi^0 \left(\frac{1-\chi}{2} Id + \frac{3\chi - 1}{2} \frac{\psi^1 \otimes \psi^1}{|\psi^1|^2} \right),$$

where χ depends only on $\frac{|\psi^1|}{\psi^0}$

[5] Levermore, *J. Stat. Phys.*, 1995

M_2 closure

$$\text{Moments} \quad \rightarrow \quad \text{ansatz} \quad \rightarrow \quad \text{closure}$$

$$(\psi^1, \psi^2) \quad \rightarrow \quad \psi_{M_2}(\Omega) \quad \rightarrow \quad \psi^3 \approx \int_{S^2} \Omega \otimes \Omega \otimes \Omega \psi_{M_2}(\Omega) d\Omega$$

Ansatz ψ_{M_2} in

$$\mathcal{C}_2 \quad = \quad \left\{ \psi \geq 0, \quad \int_{S^2} \Omega \psi d\Omega = \psi^1, \quad \int_{S^2} \Omega \otimes \Omega \psi d\Omega = \psi^2 \right\} \neq \emptyset \text{ if } \quad \boldsymbol{\psi} \in \mathcal{R}_{\mathbf{m}},$$

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[5] Levermore, *J. Stat. Phys.*, 1995

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$\hookrightarrow$ Idea: Hierarchy of approximated closure

[5] Levermore, *J. Stat. Phys.*, 1995
[6] Pichard et al, *J. Sci. Comput.* (2016)

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$\hookrightarrow \psi^3$ approximated in special cases

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$$\psi_{M_2} = \exp(S + V.\Omega + \alpha(V.\Omega)^2)$$

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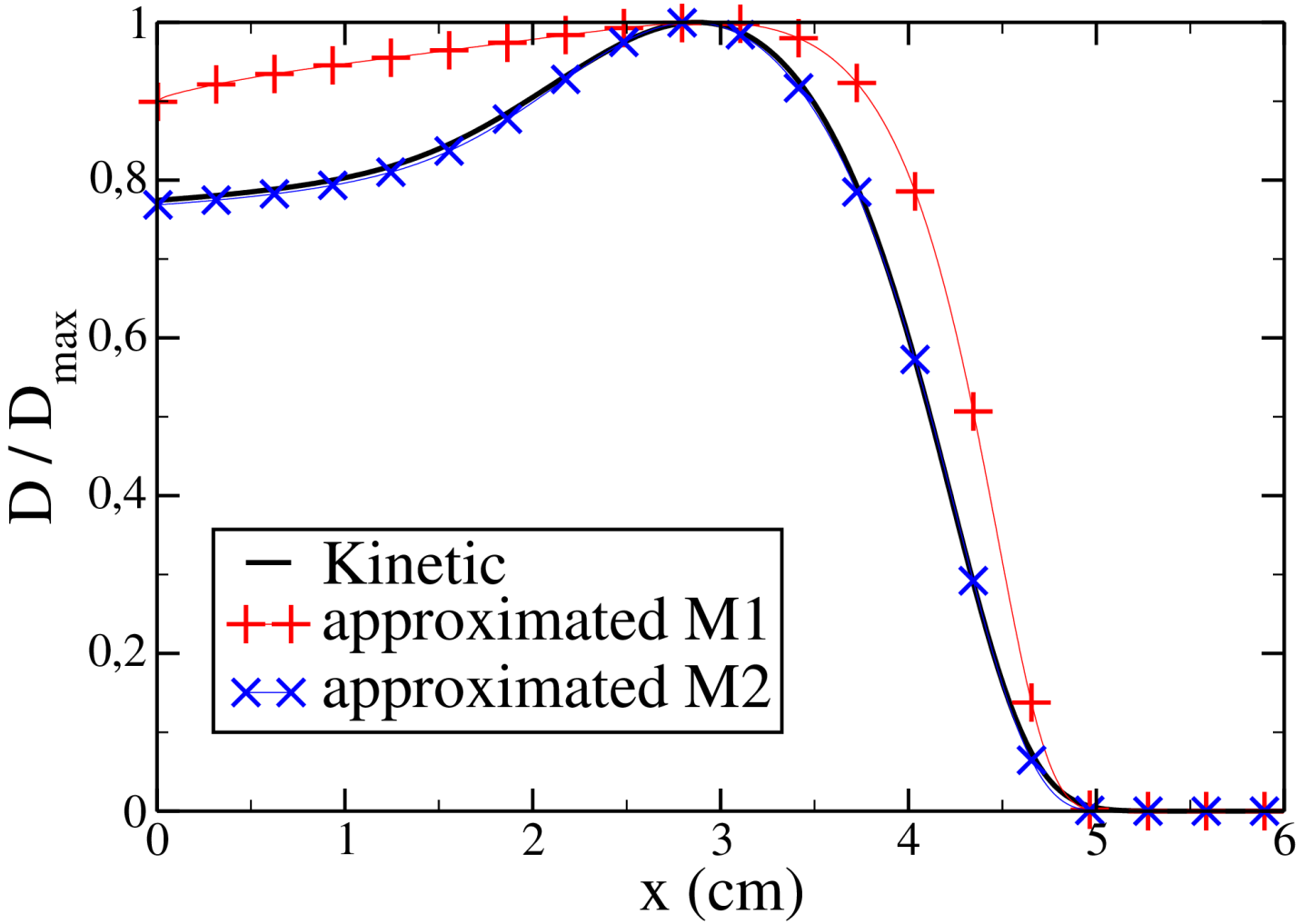
1D test case: single electron beam



Computational times: Kinetic: 30 sec; Moments: $<$ 1 sec

2D test case: double electron beam

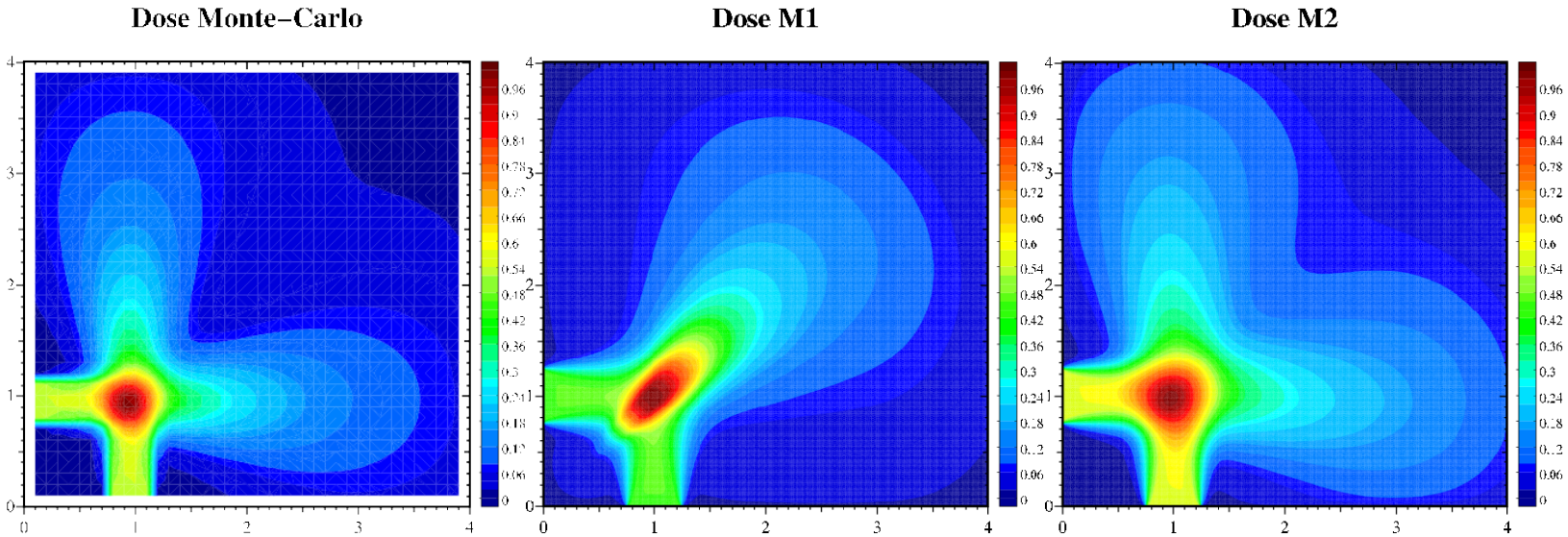


Figure : Monte Carlo PENELOPE (left), M_1 (middle), M_2 (right)

Monte Carlo: $>$ 10 h M_1: 2 min M_2: 8 min

Position of the problem

Consider

$$\partial_x \mathbf{F}(\boldsymbol{\psi}) = \rho \partial_\epsilon (S\boldsymbol{\psi})$$

HLL type numerical scheme (**backward in** ϵ)

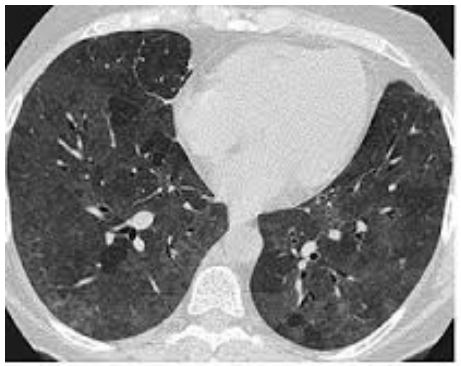
$$\frac{1}{\Delta x}\left(\frac{\mathbf{F}^n_{l+\frac{1}{2}}}{\rho_{l+\frac{1}{2}}} - \frac{\mathbf{F}^n_{l-\frac{1}{2}}}{\rho_{l-\frac{1}{2}}}\right) = \frac{S^n\boldsymbol{\psi}^n - S^{n+1}\boldsymbol{\psi}^{n+1}}{\Delta\epsilon^n}$$

$$\mathbf{F}^n_{l+\frac{1}{2}} = \frac{1}{2}\left(\mathbf{F}(\boldsymbol{\psi}^n_l) + \mathbf{F}(\boldsymbol{\psi}^n_{l+1}) - (\boldsymbol{\psi}^n_{l+1} - \boldsymbol{\psi}^n_l)\right)$$

stable under condition

$$\Delta\epsilon^n \leq S^n \Delta x \min \rho$$

very restrictive when $\rho \ll 1$

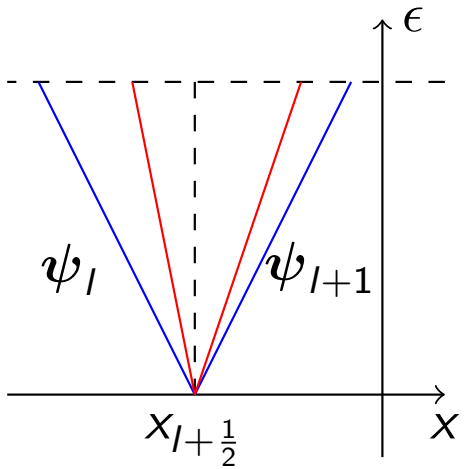


Relaxation approach in 1D[7]

Objective: Handle the non-linearity

Relaxation directions:
Define scalars $\lambda_\pm$

$$Sp(\partial_\psi \mathbf{F}(\psi)) \quad \subset \quad [\lambda_-, \lambda_+],$$



Equilibrium states:
Define vectors $\mathbf{M}_\pm(\psi)$

$$\psi = \mathbf{M}_+ + \mathbf{M}_-, \qquad \mathbf{F}(\psi) = \lambda_+ \mathbf{M}_+ + \lambda_- \mathbf{M}_-,$$

Relaxed equations:

$$\lambda_\pm \partial_x \mathbf{f}_\pm - \rho \partial_\epsilon (S \mathbf{f}_\pm) = \frac{\mathbf{M}_\pm - \mathbf{f}_\pm}{\tau},$$

Moment system $\equiv$ limit $\tau \to 0$

[7] Pichard et al, *Commun. Comput. Phys.*, 2016

Relaxation approach

Theorem (Natalini, *Commun. Pur. Appl. Math.*, 1998)

For scalar equations

$$\psi = \lim_{\tau \to 0} \mathbf{f}_+ + \mathbf{f}_-, \qquad F(\psi) = \lim_{\tau \to 0} \lambda_+ \mathbf{f}_+ + \lambda_- \mathbf{f}_-$$

Extensions:

- Parabolic equations (Bouchut, Guarguaglini and Natalini, *Indiana U. Math. J.*, 1999 ; Aregba-Driollet, Natalini and Tang, *Math. Comput.*, 2004)
- Systems (Aregba-Driollet and Natalini, *J. Numer. Anal.*, 2000)

Relaxation approach in multi-D[7]

Relaxation directions:
Define vectors λ_i

$$\forall n \in S^2, \qquad Sp(\partial_{\psi} \mathbf{F_n}(\psi)) \quad \subset \quad \left[\min_i(\lambda_i.n), \max_i(\lambda_i.n)\right],$$

Equilibrium states:
Define vectors $\mathbf{M_i}(\psi)$

$$\psi = \sum_i \mathbf{M}_i, \qquad F(\psi) = \sum_i \lambda_i \otimes \mathbf{M}_i,$$

Relaxed equations:

$$\lambda_i.\nabla_x \mathbf{f}_i - \rho \partial_{\epsilon}(S\mathbf{f}_i) = \frac{\mathbf{M}_i - \mathbf{f}_i}{\tau},$$

[7] Pichard et al, *Commun. Comput. Phys.*, 2016

Construction of a numerical scheme

1. At ϵ^n, set
$$\mathbf{f}_i^n := \mathbf{M}_i\left(\boldsymbol{\psi}^n\right)$$
2. Solve the homogeneous (**linear**) relaxed equations
$$\lambda_i . \nabla_x \mathbf{f}_i - \rho \mathbf{Q}(\mathbf{f}_i) = 0, \tag{1}$$
$$\begin{aligned} \mathbf{Q}(\mathbf{f}_i) &= \partial_\epsilon(S\mathbf{f}_i), && \rightarrow \textbf{ Explicit } \text{scheme}, \\ \mathbf{Q}(\mathbf{f}_i) &= \int_\epsilon^{\epsilon_{\max}} \boldsymbol{\sigma}(\epsilon', \epsilon)\boldsymbol{\psi}(\epsilon')d\epsilon' + \ldots, && \rightarrow \textbf{ Implicit } \text{scheme}, \end{aligned}$$
3. Project
$$\boldsymbol{\psi}^{n+1} = \sum_i \mathbf{f}_i^{n+1}$$

Construct inconditionally stable schemes for (1)

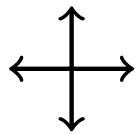
Example of relaxation parameters

In 1D:

$$\lambda_- = -1, \qquad \lambda_+ = +1, \qquad \mathbf{M}_\pm \in \mathcal{R}_\mathbf{m}$$

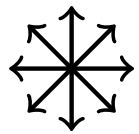
In 3D:

Cartesian: $\lambda_i = \pm 2 e_i,$



Diagonal: $\lambda_i = \pm 2 \dfrac{(e_1 \pm e_2)}{\sqrt{2}},$

Star: Cartesian + Diagonal,



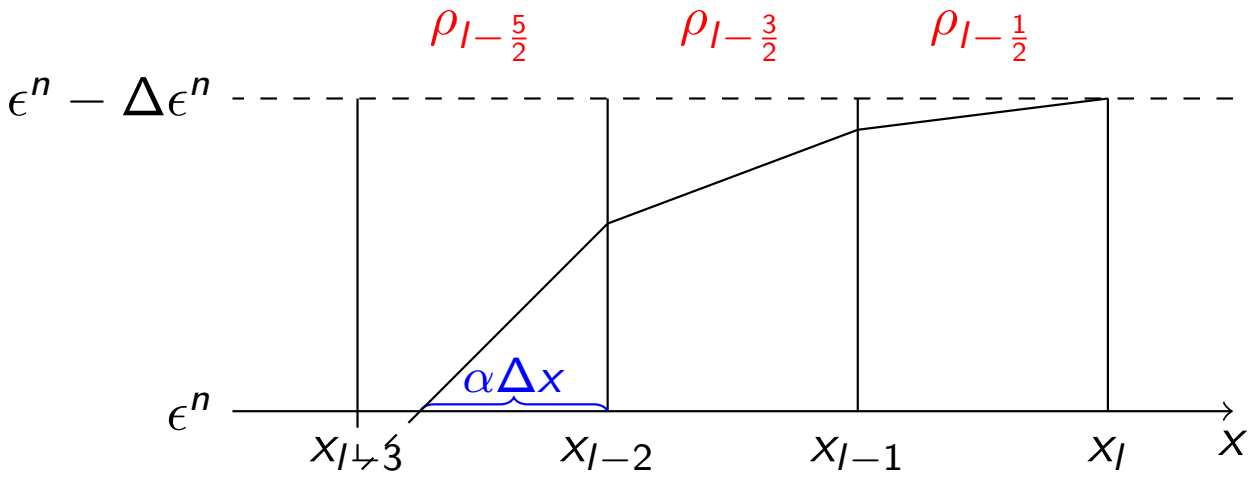
$$\mathbf{M}_i \in \mathcal{R}_\mathbf{m}$$

CFL free scheme: 1D explicit FD scheme

Simplified hyperbolic equation

$$\partial_\epsilon f + \frac{\lambda_-}{\rho(x)} \partial_x f = 0,$$

Method of characteristics



Finite Difference scheme

$$f_I^{n+1} = (1-\alpha)\, f_{I-k_I+1}^n + \alpha f_{I-k_I}^n.$$

CFL free scheme: multi-D explicit FD scheme

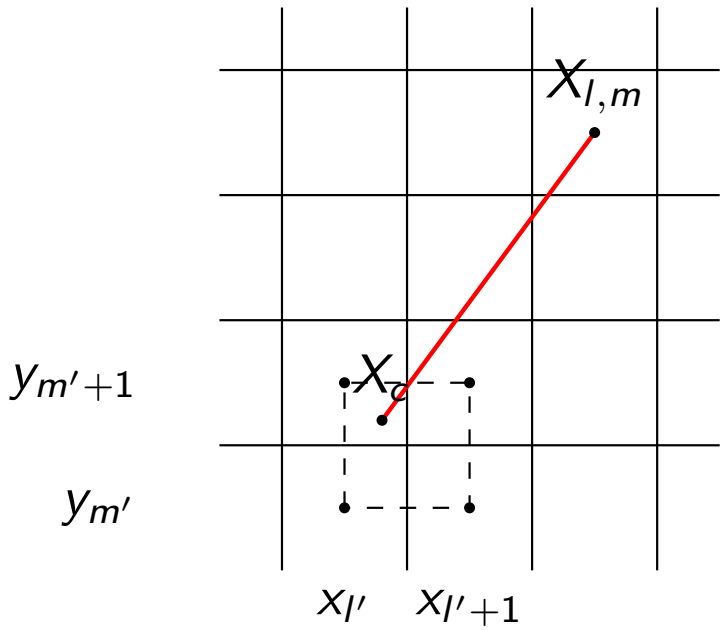
Simplified hyperbolic equation

$$\partial_\epsilon f + \frac{\lambda_i}{\rho(x)}.\nabla_x f = 0,$$

Finite Difference scheme

$$f_{l,m}^{n+1} = \sum_{i=0}^{1}\sum_{j=0}^{1} \alpha_{i,j} f_{l'+i,m'+j}^{n}.$$

Method of characteristics



1D test case: single electron beam in a heterogeneous medium

1D medium: 12 cm $\rightarrow$ 1200 cells
composed of slabs of density $\rho_{air} = 10^{-3}$ and $\rho_{water} = 1$

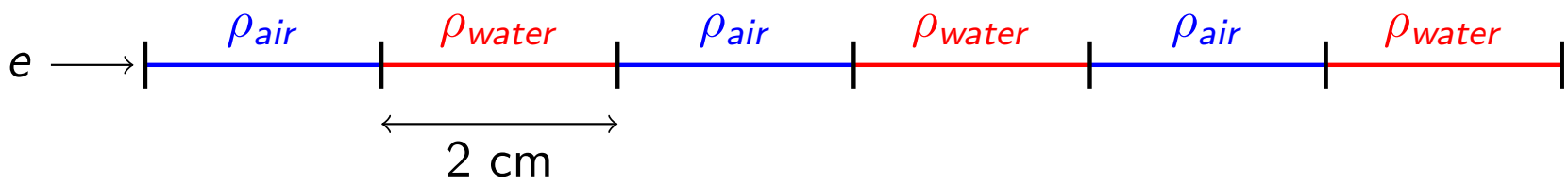


Figure : Representation of the 1D medium.

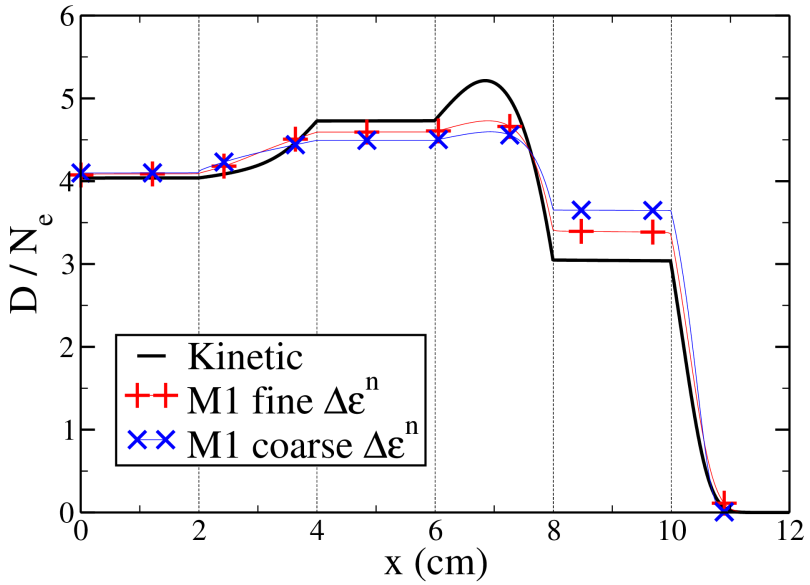
Energy step size:

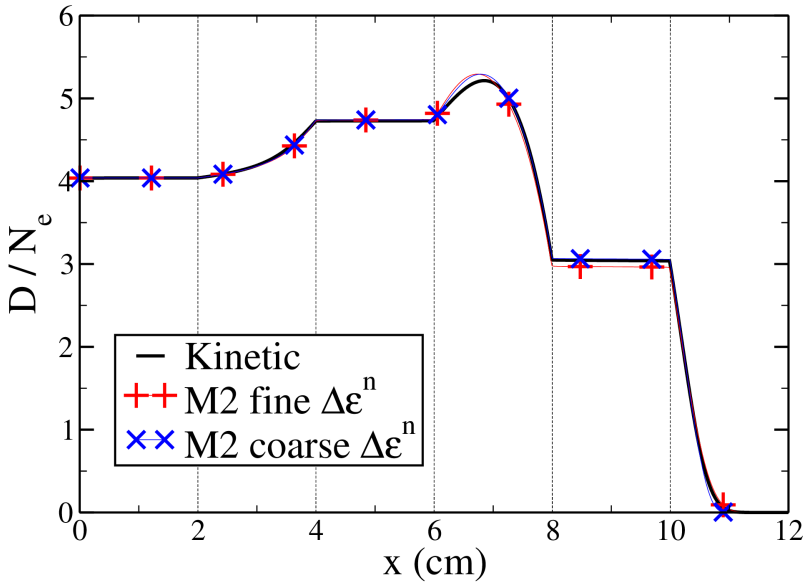
Coarse: $\Delta\epsilon^n = 0.95 S^n \rho_{water} \Delta x$,

Fine: $\Delta\epsilon^n = 0.95 S^n \rho_{air} \Delta x$

$\hookrightarrow$ equivals to HLL type solver

1D test case: single electron beam in a heterogeneous medium





Kinetic: 15 min; **Moments**: Fine steps: M_1: 20 sec, M_2: 1 min
Coarse steps: < 1 sec

2D test case: Dose in a cut of a chest

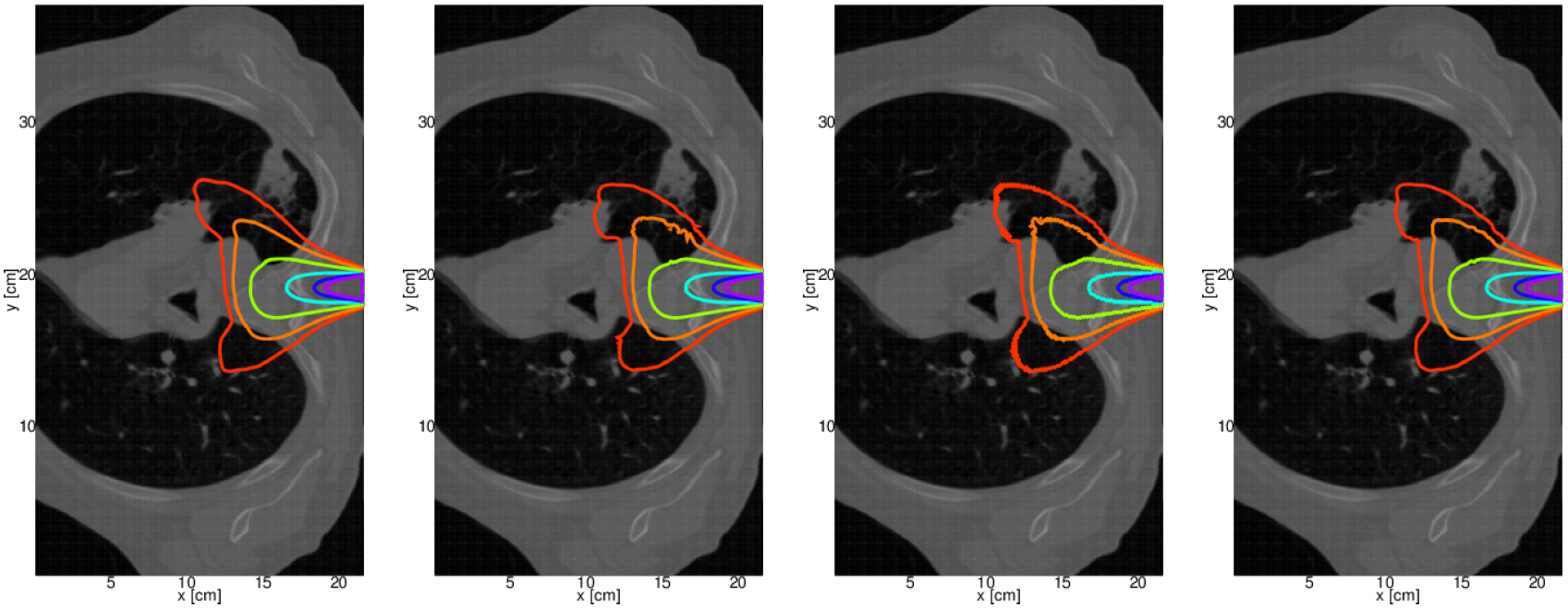


Figure : Isodose curves

Cartesian	+	fine	$\Delta\epsilon^n$	(left)	:	1 h 20 min
Cartesian	+	coarse	$\Delta\epsilon^n$	(middle left)	:	20 sec
Diagonal	+	coarse	$\Delta\epsilon^n$	(middle right)	:	22 sec
Star	+	coarse	$\Delta\epsilon^n$	(right)	:	1 min

2D test case: Error on the dose

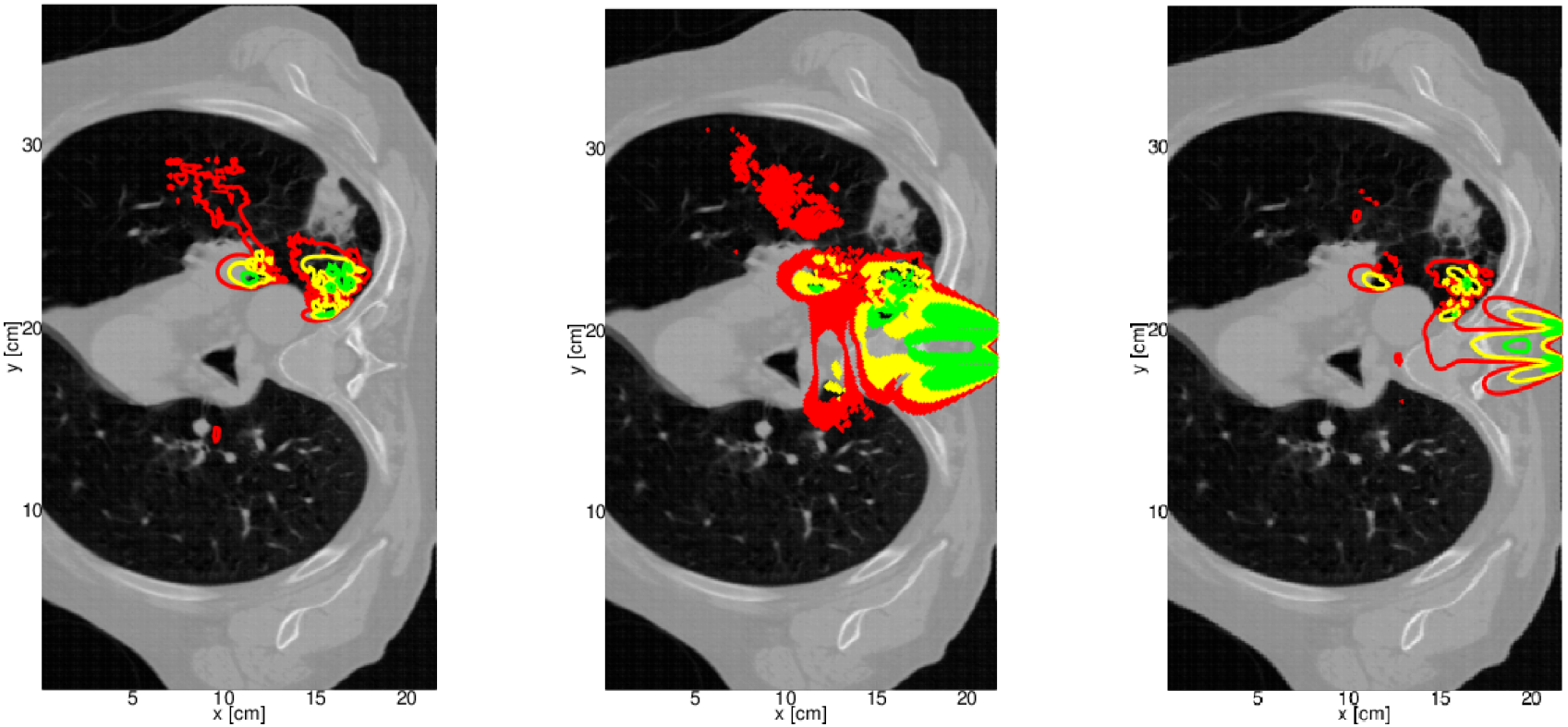


Figure : Error compared to the results with fine $\Delta\epsilon^n$

Cartesian	+	coarse	$\Delta\epsilon^n$	(left)
Diagonal	+	coarse	$\Delta\epsilon^n$	(middle)
Star	+	coarse	$\Delta\epsilon^n$	(right)

Implicit scheme

Equation

$$\partial_x \mathbf{F}(\psi) - \rho \mathbf{Q}(\psi) = 0,$$

$$\mathbf{Q}(\psi) = \int_{\epsilon}^{\epsilon_{\max}} \boldsymbol{\sigma}(\epsilon', \epsilon)\psi(\epsilon')d\epsilon' + \dots \tag{2}$$

Discretization

$$\frac{1}{\Delta x}\left(\frac{\mathbf{F}_{l+\frac{1}{2}}^{n+1}}{\rho_{l+\frac{1}{2}}} - \frac{\mathbf{F}_{l-\frac{1}{2}}^{n+1}}{\rho_{l-\frac{1}{2}}}\right) - \mathbf{Q}_l^{n+1} = 0,$$

$$\mathbf{F}_{l+\frac{1}{2}}^{n+1} = \frac{1}{2}\left(\mathbf{F}(\psi_l^{n+1}) + \mathbf{F}(\psi_{l+1}^{n+1}) - (\psi_{l+1}^{n+1} - \psi_l^{n+1})\right),$$

(2) discretized with: **Quadrature** + ...

$$\mathbf{Q}_l^{n+1} = A^{n+1,n+1}\psi_l^{n+1} + \underbrace{\sum_{n'=1}^{n} A^{n',n+1}\psi_l^{n'}}_{\mathbf{U}_l^n}$$

An Implicit numerical scheme

Discretization

$$\frac{1}{\Delta x}\left(\frac{\mathbf{F}_{l+\frac{1}{2}}^{n+1}}{\rho_{l+\frac{1}{2}}}-\frac{\mathbf{F}_{l-\frac{1}{2}}^{n+1}}{\rho_{l-\frac{1}{2}}}\right)-A^{n+1,n+1}\boldsymbol{\psi}_l^{n+1}=\mathbf{U}_l^n, \tag{3}$$

Proposition

If for all $k \geq 0$ and l

$$\boldsymbol{\psi}_l^{n-k} \in \mathcal{R}_{\mathbf{m}}^2,$$

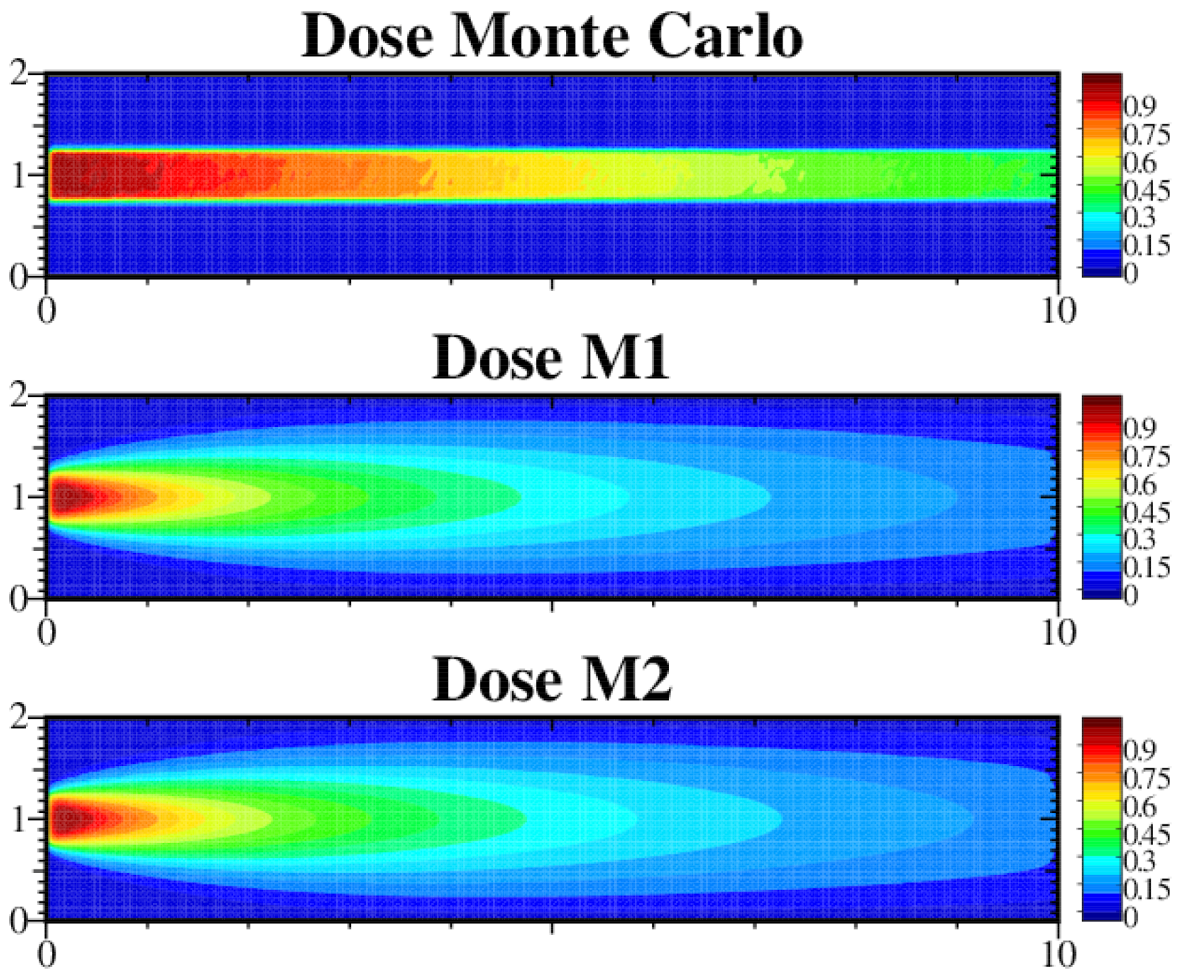
then there exists a unique solution

$$\boldsymbol{\psi}_l^{n+1} \in \mathcal{R}_{\mathbf{m}}^2 \qquad \text{for all } l$$

to (3).

$\hookrightarrow$ contraction method

2D test case: single photon beam



Monte Carlo: 14 h; M_1: 50 sec M_2: 215 sec

2D test case: single photon beam

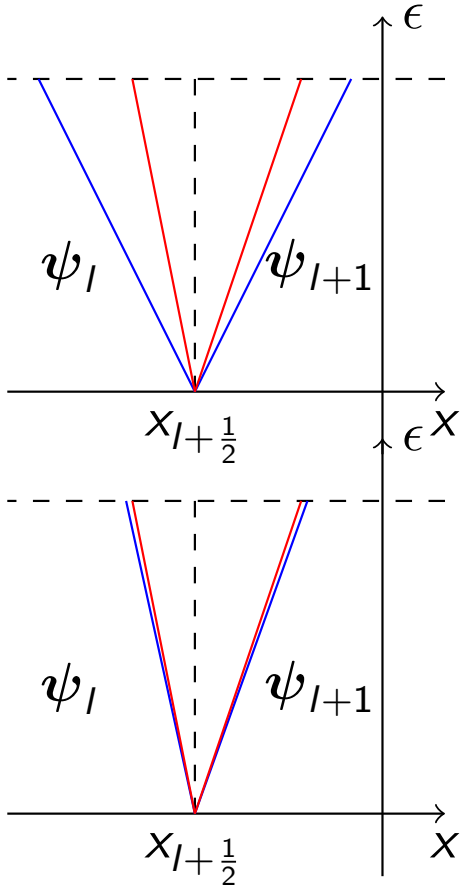
Constraints:

$$Sp(\partial_\psi \mathbf{F_n}(\psi)) \subset \left[\min_i(\lambda_i.n), \max_i(\lambda_i.n)\right] \tag{4}$$

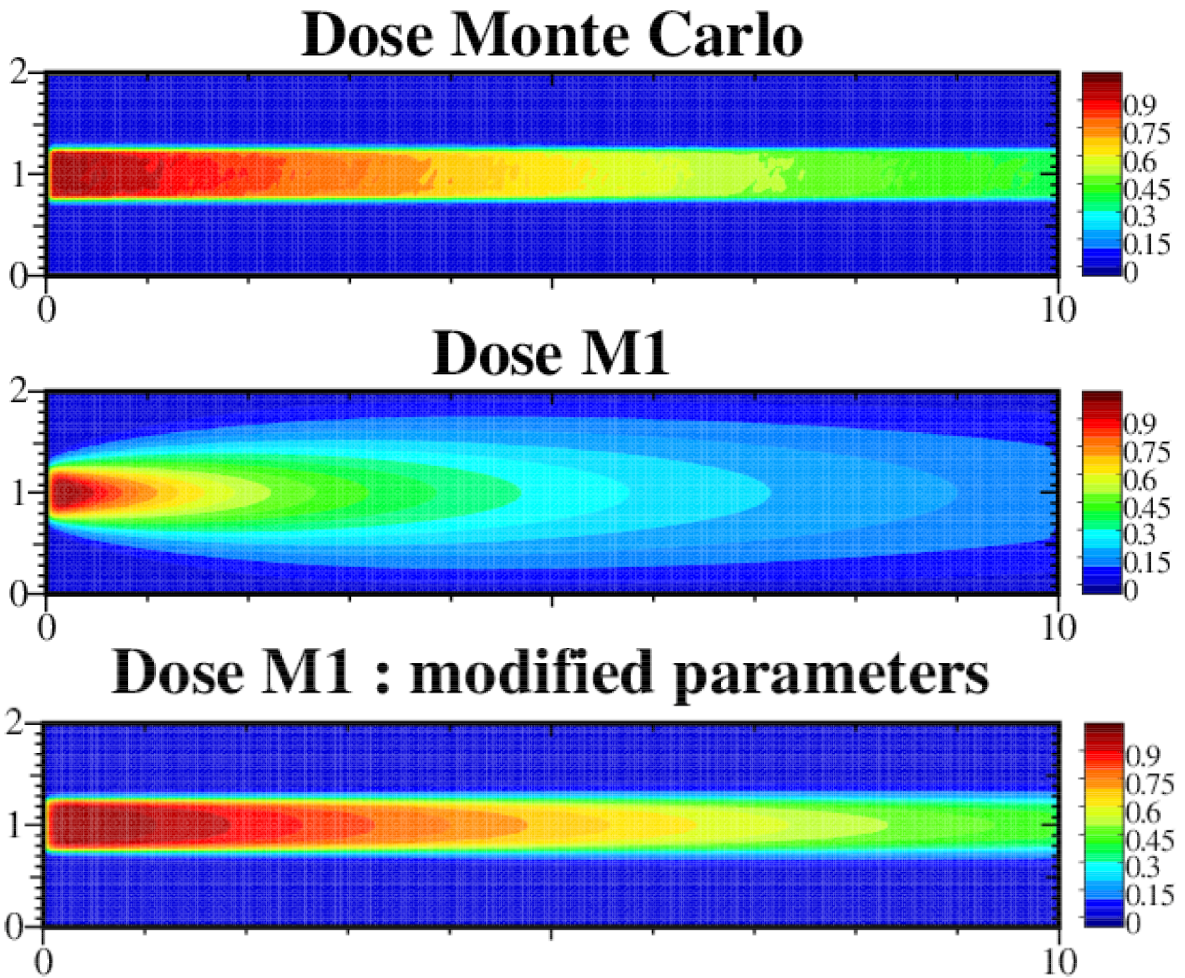
Relaxation parameters:

Non-modified: $\lambda_i = \pm 2 e_i,$

Modified: $\lambda_i = \pm|\lambda_i| e_i,$ s.t. (4)

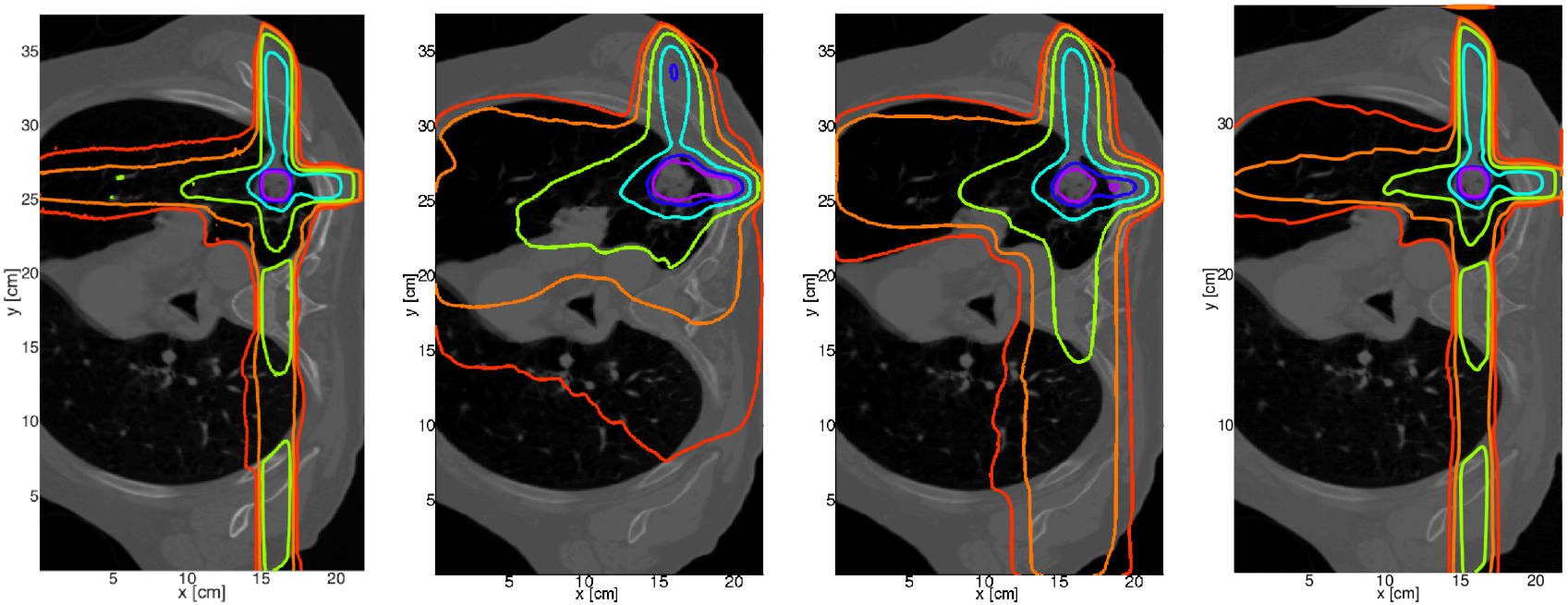


2D test case: single photon beam



Monte Carlo: 14 h; Non-modified: 50 sec Modified: 205 sec

2D test case: double photon beam in a chest



Monte Carlo (left)	:	14 h
M_1 Non-modified (middle left)	:	13 min
M_2 Non-modified (middle right)	:	30 min
M_1 Modified (right)	:	24 min

Conclusion

Problems

- Computation of the closure
- Numerical scheme with a non-linear term
- Numerical scheme with a stiff term

Solutions

- Approximation of the closure
- Relaxation method
- Implicit scheme inconditionally stable

Perspectives

Numerical scheme

- Higher order method
- Bounding of the eigenvalues of the Jacobian of the M_2 flux

Physics

- Consider more collision types
- Radiobiology

Moment problem

- Characterizing realizability
- Construct other closures

Optimization

- Improve algorithm

Thanks for your attention

Method of moments

Astrophysics:

- Chandrasekhar (1944-1960)

Radiative transfer:

- Minerbo (1977-1978)
- Dubroca, Feugeas (1999)
- Buet, Després (2006)

Fluid:

- Grad (1949)
- Levermore (1996)

Plasma physics:

- Mallet, Brull, Dubroca (2014, 2015)
- Guisset, Brull, d'Humières, Dubroca, Tikhonchuk (2016)

Semi-conductors:

- Anile, Romano (2000)
- Hauck (2006)

Chemotaxy:

- Borsche, Klar, Pham (2016)

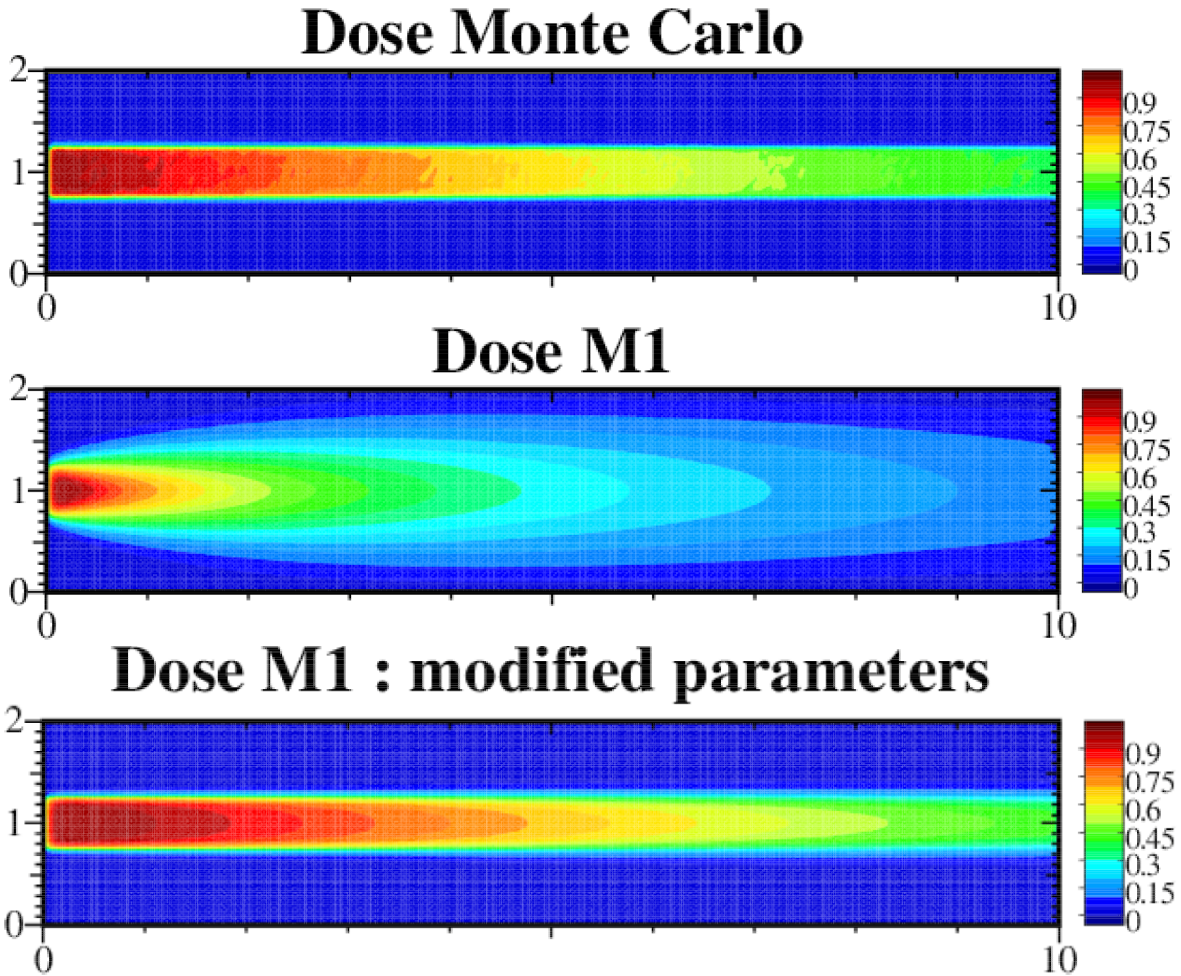
Radiotherapy:

- Duclous, Dubroca, Frank (2010)
- Olbrant, Frank (2010)
- Present PhD thesis (2016)

Others:

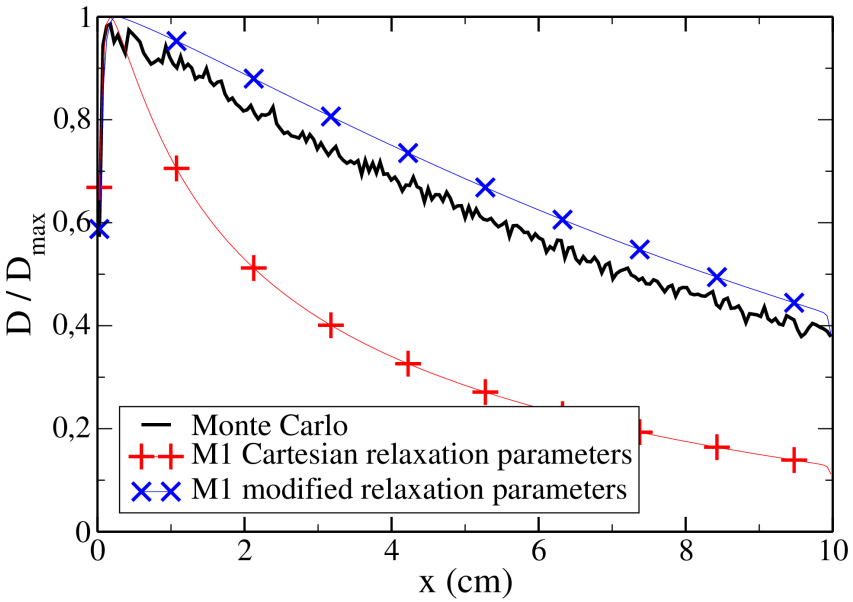
- Junk (2000)
- Schneider (2004)
- Hauck, Levermore, Tits (2007)
- Alldredge, Hauck, Tits (2012)

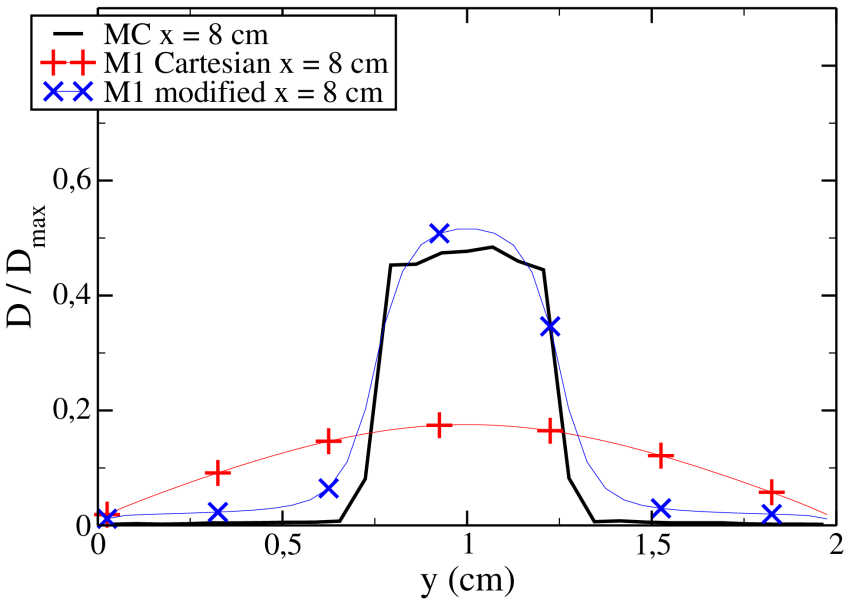
2D test case: single photon beam



Monte Carlo: 14 h; Non-modified: 50 sec Modified: 205 sec

2D test case: single photon beam





Monte Carlo: 14 h; Non-modified: 50 sec Modified: 205 sec

Optimization problem

Objectif: minimize

$$J(\psi, \psi^b) = \|D(\psi) - \bar{D}\|_Z^2 + \alpha \|\psi^b\|_{\partial Z}^2$$

Direct equations

$$\begin{cases} \Omega.\nabla_x \psi &= Q(\psi), \\ \psi &= \psi^b \quad \text{on } \Gamma^- \\ \psi(\epsilon = \epsilon_{\max}) &= 0 \end{cases}$$

Optimization procedure

Lagrangian

$$L(\psi^b, \psi, \lambda, \lambda^b) = J(\psi^b, \psi) - (\psi - \psi^b, \lambda^b)_{\Gamma^-} - (\Omega.\nabla_x \psi - Q(\psi), \lambda)_{Int}$$

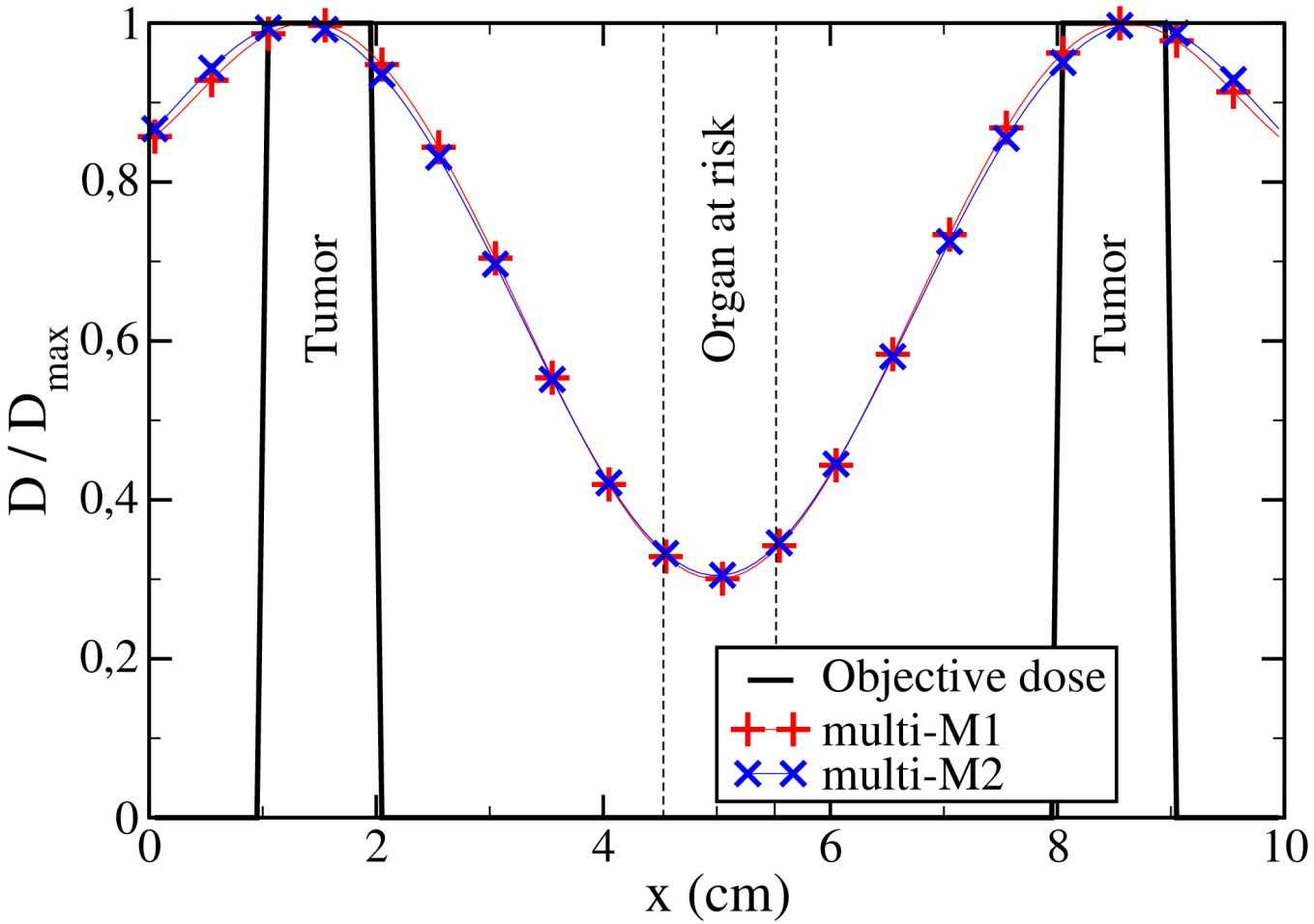
Differentiating

$$\begin{aligned}
d_\lambda L(\psi, \psi^b, \lambda, \lambda^b)(h) &= (\Omega.\nabla_x \psi - Q(\psi),\ h)_{Int}\,, \\
d_{\lambda^b} L(\psi, \psi^b, \lambda, \lambda^b)(h) &= \left(\psi - \psi^b,\ h\right)_{\Gamma^-}\,, \\
d_\psi L(\psi, \psi^b, \lambda, \lambda^b)(h) &= \left(-\Omega.\nabla_x \lambda - Q^T(\lambda) + f(\psi),\ h\right)_{Int} \\
&\quad -(\lambda - \lambda^b,\ h)_{\Gamma^-} + (\lambda,\ h)_{\Gamma^+} + (g(\lambda), h)_{\epsilon_{\max}}, \\
d_{\psi^b} L(\psi, \psi^b, \lambda, \lambda^b)(h) &= (\alpha\psi^b - \lambda^b,\ h)_{\Gamma^-} = d_{\psi^b} J(\Xi(\psi^b), \psi^b),
\end{aligned}$$

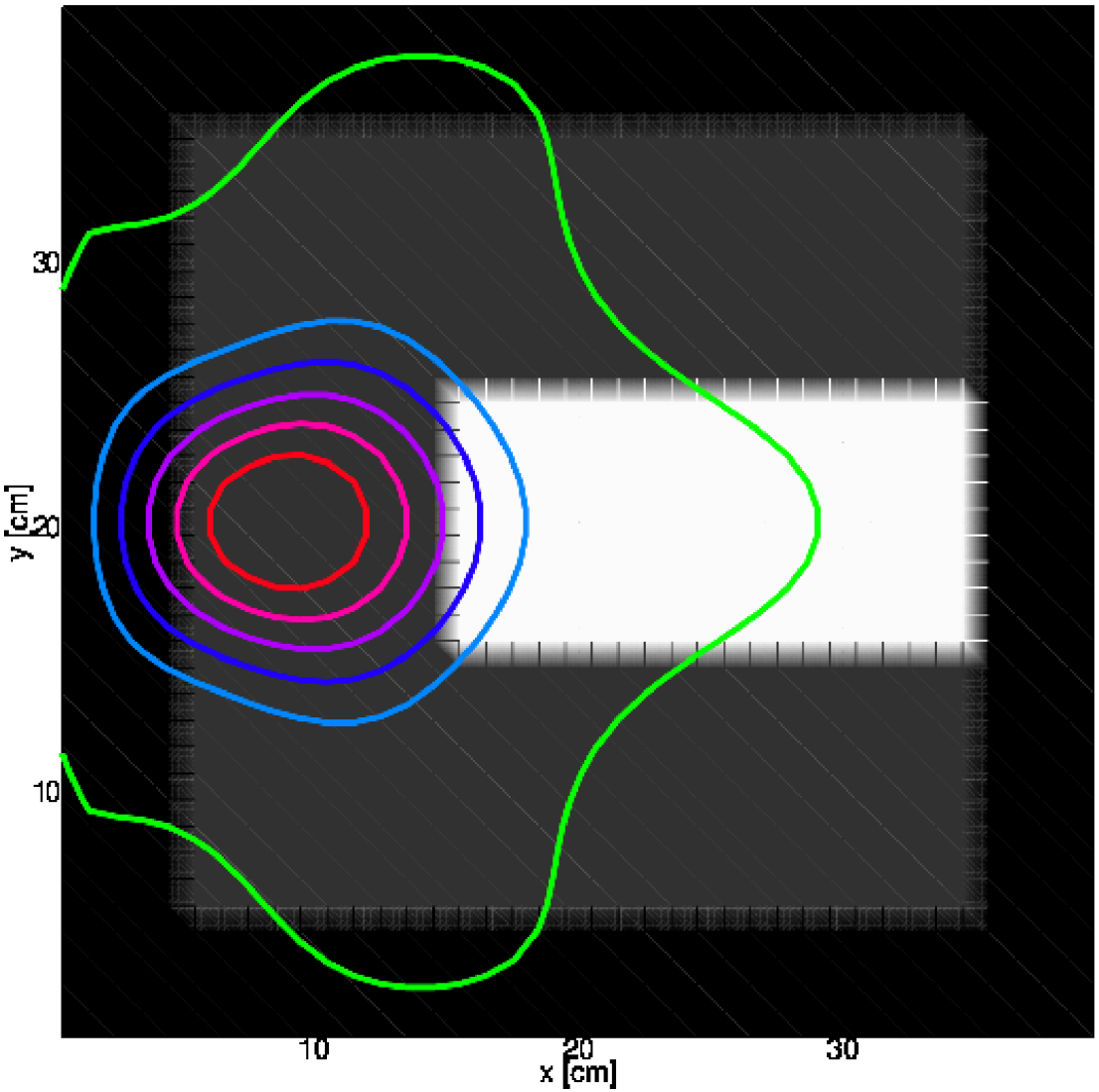
Adjoint equation

$$\begin{cases}
-\Omega.\nabla_x \lambda &= Q^T(\lambda) + f(\psi), \\
\lambda &= 0 \quad \text{on } \Gamma^+ \\
\lambda(\epsilon = \epsilon_{\min}) &= 0
\end{cases}$$

Optimization results: 1D



Optimization results: 2D with M_1



Optimization results: 2D with M_2