The M_1 and M_2 models for dose computation in radiotherapy

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Context

Objective : destruction of tumor cells
Method : ionizing radiations

Models

- **Kinetic approach**
  ↪ numerically too costly
- **Angular moment approach**
  ↪ numerical challenge
- **Hydrodynamic approach**
  ↪ inaccurate

1. Kinetic model

2. Moment model

3. Numerical results

Kinetic model

Fluence : $\psi = |v| f$
spherical coordinates $v = |v|(\epsilon)\Omega$

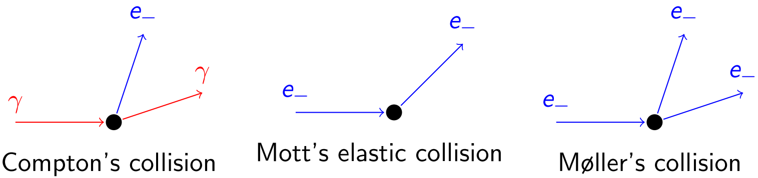
[1] *Hensel et al, Phys. Med. Biol., 2006*
[2] *Pomraning, Math. Mod. Meth. Appl. S., 1992*

Kinetic model

Fluence : $\psi = |v| f$
spherical coordinates $v = |v|(\epsilon)\Omega$

Stationnary kinetic equations[1,2]

$$\begin{aligned}
\Omega.\nabla_x \psi_\gamma &= \rho \left[G_{\gamma\to\gamma}(\psi_\gamma) - \sigma_{T,\gamma}\psi_\gamma \right], \\
\Omega.\nabla_x \psi_e &= \rho \left[\partial_\epsilon (S\psi_e) + G_{e\to e}(\psi_e) + G_{\gamma\to e}(\psi_\gamma) - \sigma_{T,e}\psi_e \right], \\
G_{i\to j}(\psi_i) &= \int_{S^2}\int_\epsilon^\infty \sigma_{i\to j}(\epsilon', \epsilon, \Omega'.\Omega)\psi_i(x, \epsilon', \Omega') d\epsilon' d\Omega'.
\end{aligned}$$

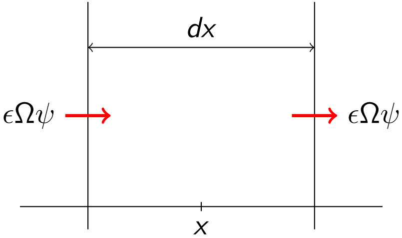


[1] *Hensel et al, Phys. Med. Biol., 2006*
[2] *Pomraning, Math. Mod. Meth. Appl. S., 1992*

Kinetic model

Dose : energy transfered at point x

$$
\begin{aligned}
D(x) &= \int_{\epsilon=0}^{+\infty} S(\epsilon)\psi_e^0(x,\epsilon)d\epsilon, \\
\psi^0 &= \int_{\Omega\in S^2} \psi(x,\Omega,\epsilon)d\Omega
\end{aligned}
$$



1. Kinetic model
2. Moment model
3. Numerical results

Method of moments

Fluid/Hydrodynamic:

- Grad (1949)
- Levermore (1995)

Plasma physics:

- Mallet, Brull, Dubroca (2013)
- Guisset, Brull, D'Humière, Dubroca, Karpov, Potapenko (2015)

Semi-conductors:

- Anile, Romano (2000)

Radiative transfer:

- Minerbo (1977-1978)
- Dubroca, Feugeas (1999)

Radiotherapy:

- Duclous, Dubroca, Frank (2010)
- Olbrant, Frank (2010)

Others:

Alldredge, Hauck, Tits (2012)
Hauck, Levermore, Tits (2007)

Moments

Aim : reduce computational costs

Moments methods:

$$\psi(x,\epsilon,\Omega) \quad \leftrightarrow \quad \psi^i(x,\epsilon) \quad \text{for} \quad 0 \leq i \leq N$$

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

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

M_1 equations

Orders 0 and 1

$$\gamma \quad \begin{cases} \nabla_x . \psi_\gamma^1 = \rho \left[G^0_{\gamma\to\gamma}(\psi_\gamma^0) - \sigma_{T,\gamma}\psi_\gamma^0 \right] \\ \nabla_x . \psi_\gamma^2 = \rho \left[G^1_{\gamma\to\gamma}(\psi_\gamma^1) - \sigma_{T,\gamma}\psi_\gamma^1 \right] \end{cases}$$

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

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$\hookrightarrow$ requires a closure

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

M_1 closure

Moments

(ψ^0, ψ^1)

M_1 closure

Moments → ansatz

$(\psi^0, \psi^1) \quad \rightarrow \quad \psi_{M_1}(\Omega)$

Ansatz ψ_{M_1} in

$$\mathcal{C}_1 = \left\{ \psi \geq 0, \quad \int_{S^2} \psi d\Omega = \psi^0, \quad \int_{S^2} \Omega \psi d\Omega = \psi^1 \right\} \neq \emptyset,$$

M_1 closure

Moments $\rightarrow$ ansatz $\rightarrow$ closure

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

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Choice of the ansatz[3,4]

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

[3] *Minerbo, QSRT, 1977*

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

M_1 closure

M_1 closure:

$$\psi_{M_1} = \exp\left(S + V.\Omega\right) \quad \rightarrow \quad \psi^2 \approx \int_{S^2} \Omega \otimes \Omega \psi_{M_1} d\Omega.$$

Numerical costs:

$\hookrightarrow$ minimization problem

$\hookrightarrow$ numerical quadrature

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Alternative computation:

$$\psi^2 = \psi^0 \left(\frac{1-\chi}{2} Id + \frac{3\chi - 1}{2} \frac{\psi^1 \otimes \psi^1}{||\psi^1||_2^2} \right),$$

where χ depends only on $\frac{||\psi^1||_2}{\psi^0}$

M_2 model

Remark:

$$tr(\Omega \otimes \Omega) = ||\Omega||_2^2 = 1 \quad \Rightarrow \quad tr(\psi^2) = \psi^0$$

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Orders 1 and 2

$$\gamma \quad \begin{cases} \nabla_x . \psi_\gamma^2 = \rho \left[G^1_{\gamma\to\gamma}(\psi_\gamma^1) - \sigma_{T,\gamma}\psi_\gamma^1 \right] \\ \nabla_x . \psi_\gamma^3 = \rho \left[G^2_{\gamma\to\gamma}(\psi_\gamma^2) - \sigma_{T,\gamma}\psi_\gamma^2 \right] \end{cases}$$

$$e_- \quad \begin{cases} \nabla_x . \psi_e^2 = \rho \left[\partial_\epsilon(S\psi_e^1) + G^1_{e\to e}(\psi_e^1) + G^1_{\gamma\to e}(\psi_\gamma^1) - \sigma_{T,e}\psi_e^1 \right] \\ \nabla_x . \psi_e^3 = \rho \left[\partial_\epsilon(S\psi_e^2) + G^2_{e\to e}(\psi_e^2) + G^2_{\gamma\to e}(\psi_\gamma^2) - \sigma_{T,e}\psi_e^2 \right] \end{cases}$$

$\hookrightarrow$ requires a closure

$$\psi_\gamma^3 = g_\gamma(\psi_\gamma^1, \psi_\gamma^2), \quad \psi_e^3 = g_e(\psi_e^1, \psi_e^2)$$

M_2 closure

Moments → ansatz → closure

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

Ansatz ψ_{M_2} in

$$\mathcal{C}_2 = \left\{ \psi \geq 0, \quad \int_{S^2} \Omega \psi d\Omega = \psi^1, \quad \int_{S^2} \Omega \otimes \Omega \psi d\Omega = \psi^2 \right\} \neq \emptyset,$$

Choice of the ansatz[4,5]

$$\psi_{M_2} = \underset{\psi \in \mathcal{C}_2}{argmin}(\mathcal{H}(\psi)) \quad \Rightarrow \quad \psi_{M_2} = \exp\left(V.\Omega + M : \Omega \otimes \Omega\right),$$

[4] *Minerbo, QSRT, 1977*

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

M_2 closure

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Numerical cost:

$\hookrightarrow$ minimization problem

$\hookrightarrow$ numerical quadrature

[6] *P., Alldredge, Brull, Dubroca, Frank, submitted*

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Alternative: approximation[6]

↪ Idea: Hierarchy of approximated closure

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Numerical cost:

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Alternative: approximation[6]

↪ Idea: Hierarchy of approximated closure

↪ ψ^3 approximated in special cases

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

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Numerical cost:

↪ minimization problem

↪ numerical quadrature

Alternative: approximation[6]

↪ Idea: Hierarchy of approximated closure

↪ ψ^3 approximated in special cases

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

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M_2 closure

M_2 closure:

$$\psi_{M_2} = \exp\left(V.\Omega + M : \Omega \otimes \Omega \right) \quad \rightarrow \quad \psi^3 \approx \int_{S^2} \Omega \otimes \Omega \otimes \Omega \psi_{M_2} d\Omega.$$

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1. Kinetic model
2. Moment model
3. Numerical results

Numerical approach: kinetic

Kinetic equations:

$$\begin{aligned}
\Omega.\nabla_x\psi_\gamma &= \rho\left[G_{\gamma\to\gamma}(\psi_\gamma) - \sigma_{T,\gamma}\psi_\gamma\right],\\
\Omega.\nabla_x\psi_e &= \rho\left[\partial_\epsilon(S\psi_e) + G_{e\to e}(\psi_e) + G_{\gamma\to e}(\psi_\gamma) - \sigma_{T,e}\psi_e\right],\\
G_{i\to j}(\psi_i) &= \int_{S^2}\int_\epsilon^\infty \sigma_{i\to j}(\epsilon',\epsilon,\Omega'.\Omega)\psi_i(x,\epsilon',\Omega')d\epsilon' d\Omega'.
\end{aligned}$$

solving backward : from ϵ_{max} to 0

Method for kinetic equations :

↪ Upwind schemes in 1D

↪ Monte-Carlo in 2D

Numerical approach

M_1 equations

$$\gamma \quad \begin{cases} \nabla_x.\psi_\gamma^1 = \rho\left[G^0_{\gamma\to\gamma}(\psi^0_\gamma) - \sigma_{T,\gamma}\psi^0_\gamma\right] \\ \nabla_x.\psi_\gamma^2 = \rho\left[G^1_{\gamma\to\gamma}(\psi^1_\gamma) - \sigma_{T,\gamma}\psi^1_\gamma\right] \end{cases}$$

$$e_- \quad \begin{cases} \nabla_x.\psi_e^1 = \rho\left[\partial_\epsilon(S\psi^0_e) + G^0_{e\to e}(\psi^0_e) + G^0_{\gamma\to e}(\psi^0_\gamma) - \sigma_{T,e}\psi^0_e\right] \\ \nabla_x.\psi_e^2 = \rho\left[\partial_\epsilon(S\psi^1_e) + G^1_{e\to e}(\psi^1_e) + G^1_{\gamma\to e}(\psi^1_\gamma) - \sigma_{T,e}\psi^1_e\right] \end{cases}$$

solving backward : from ϵ_{max} to 0

Method for moment equations :

$\hookrightarrow$ Numerical scheme[5,6] based on relaxation method[7,8]

[5] *P., Alldredge, Brull, Dubroca, Frank, submitted*

[6] *P., Aregba-Driollet, Brull, Dubroca, Frank, to appear in CiCP*

[7] *Natalini, J. Eqt. Dif., 1998*

[8] *Aregba-Driollet, Natalini, SIAM J. Numer. Anal., 2000*

Numerical approach

M_2 equations

$$\gamma \quad \begin{cases} \nabla_x . \psi_\gamma^2 = \rho\left[G^1_{\gamma\to\gamma}(\psi_\gamma^1) - \sigma_{T,\gamma}\psi_\gamma^1\right] \\ \nabla_x . \psi_\gamma^3 = \rho\left[G^2_{\gamma\to\gamma}(\psi_\gamma^2) - \sigma_{T,\gamma}\psi_\gamma^2\right] \end{cases}$$

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1D test case : single electron beam

1D medium : 6cm $\rightarrow$ 600 cells

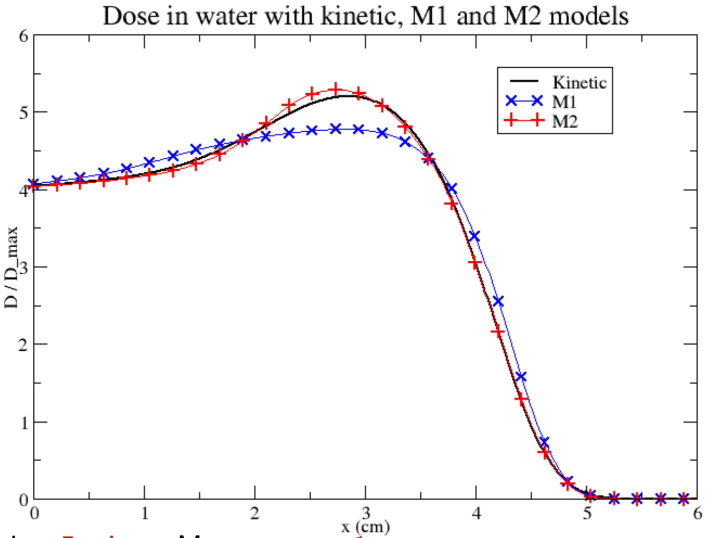
Initial condition :

$$\psi_\gamma(x,\Omega,11MeV)=0,\quad \psi_e(x,\Omega,11MeV)=0,$$

Boundary condition :

$$\begin{aligned}
\psi_\gamma(x=0cm,\Omega,\epsilon) &= \psi_\gamma(x=6cm,\Omega,\epsilon)=0,\\
\psi_e(x=0cm,\Omega,\epsilon) &= 10^{10}\exp\left(-\frac{(\epsilon-\mathbf{10MeV})^2}{(0.05\epsilon_0)^2}\right)\\
&\qquad \exp\left(-1000(1-\Omega.e_1)^2\right) \quad \text{for } \Omega.e_1>0,\\
\psi_e(x=6cm,\Omega,\epsilon) &= 0, \qquad\qquad \text{for } \Omega.e_1<0.
\end{aligned}$$

1D test case : single electron beam



Kinetic : 5 min; Moments : < 1 sec

2D test case : single photon beam

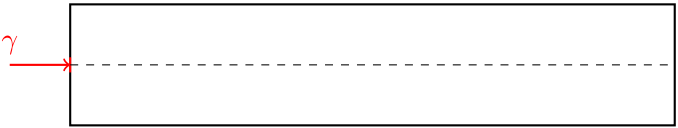
2D medium : 40cm $\times$ 8cm $\rightarrow$ 400 $\times$ 80 cells

Initial condition :

$$\psi_\gamma(x, \Omega, 1.1MeV) = 0, \quad \psi_e(x, \Omega, 1.1MeV) = 0,$$

Boundary condition :

$$\begin{aligned}
\psi_\gamma(x = 0cm, \Omega, \epsilon) &= 10^{10}\mathbf{1}_{[3.5cm,4.5cm]}(y) \exp\left(-\frac{(\epsilon - \mathbf{1MeV})^2}{(0.05\epsilon_0)^2}\right) \\
&\quad \exp\left(-1000(1 - \Omega.e_1)^2\right) \quad \text{for } \Omega.e_1 > 0, \\
\psi_\gamma(x, \Omega, \epsilon) &= 0, \quad \text{on the other boundaries,} \\
\psi_e(x, \Omega, \epsilon) &= 0 \quad \text{on the boundaries}
\end{aligned}$$



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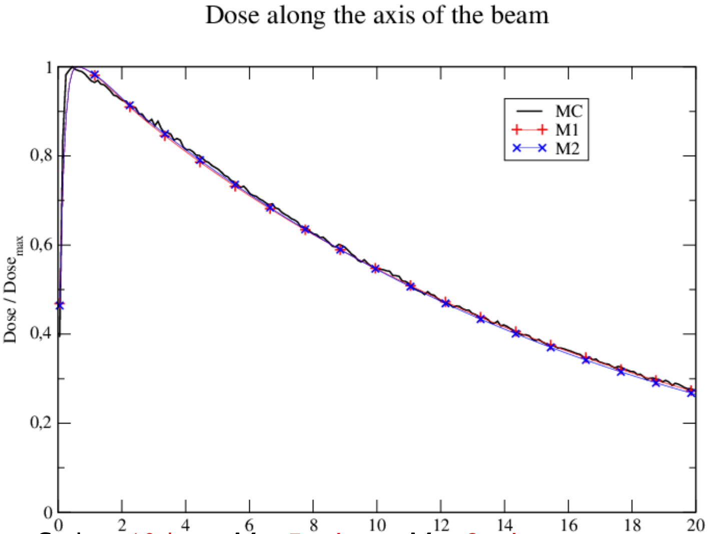

Monte-Carlo : 10 h; M_1: 5 min; M_2: 6 min

2D test case : double electron beam

2D medium : 6cm $\times$ 6cm $\rightarrow$ 600 $\times$ 600 cells
Initial condition :

$$\psi_\gamma(x,\Omega,11MeV) = 0, \quad \psi_e(x,\Omega,11MeV) = 0,$$

Boundary condition :

$$\begin{aligned}
\psi_\gamma(x,\Omega,\epsilon) &= 0, \\
\psi_e(x=0cm,\Omega,\epsilon) &= 10^{10}\mathbf{1}_{[0.75cm,1.25cm]}(y)\exp\left(-\frac{(\epsilon-\mathbf{10MeV})^2}{(0.05\epsilon_0)^2}\right) \\
&\quad \exp\left(-1000(1-\Omega.e_1)^2\right) \quad \text{for } \Omega.e_1>0, \\
\psi_e(y=0cm,\Omega,\epsilon) &= 10^{10}\mathbf{1}_{[0.75cm,1.25cm]}(x)\exp\left(-\frac{(\epsilon-\mathbf{10MeV})^2}{(0.05\epsilon_0)^2}\right) \\
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2D test case : double electron beam

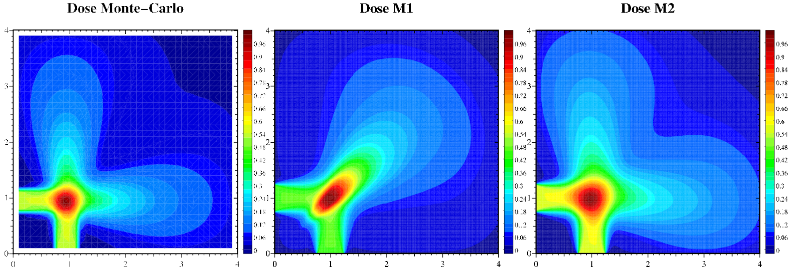

Figure : Dose with PENELOPE (Monte-Carlo, left), M_1 (middle), M_2 (right) solvers

Monte-Carlo : 14 h; M_1 : 5 min; M_2 : 14 min

2D test case : single electron beam in a chest

2D medium : 21.8cm × 37.5cm → 218 × 375 cells

Initial condition :

$$\psi_\gamma(x, \Omega, 11MeV) = 0, \quad \psi_e(x, \Omega, 11MeV) = 0,$$

Boundary condition :

$$\begin{aligned}
\psi_\gamma(x, \Omega, \epsilon) &= 0, \\
\psi_e(x = 21.8cm, \Omega, \epsilon) &= 10^{10}\mathbf{1}_{[18.25cm, 19.25cm]}(y) \exp\left(-\frac{(\epsilon - \mathbf{10MeV})^2}{(0.05\epsilon_0)^2}\right) \\
&\quad \exp\left(-1000(1 + \Omega.e_1)^2\right) \quad \text{for } \Omega.e_1 < 0, \\
\psi_e(x, \Omega, \epsilon) &= 0, \qquad \text{on the other boundaries,}
\end{aligned}$$

2D test case : single electron beam in a chest

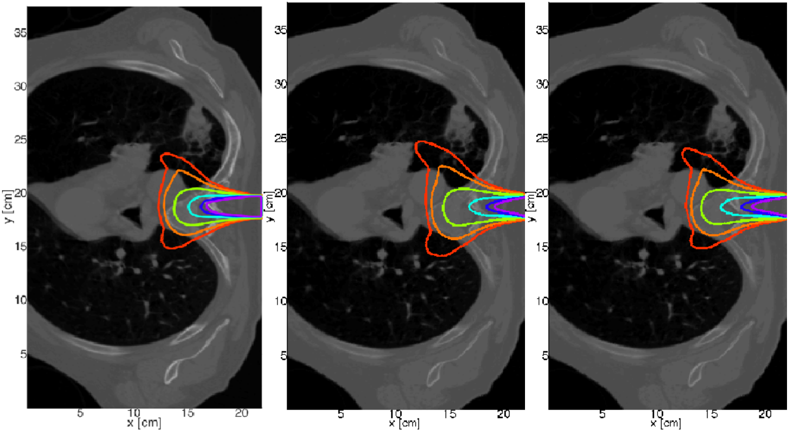

Figure : Isodose curves with PENELOPE (Monte-Carlo, left), M_1 (middle), M_2 (right) solvers

Monte-Carlo : 14 h; M_1 : 4 min; M_2 : 15 min

Conclusion and perspectives

Conclusion:

- Kinetic model : Numerically difficult
- Moments : Fast and good behavior
  $\hookrightarrow$ M_1 model : faster but miss some effects
  $\hookrightarrow$ M_2 model : capture more physical phenomena

Conclusion and perspectives

Conclusion:

- Kinetic model : Numerically difficult
- Moments : Fast and good behavior
  ↪ M_1 model : faster but miss some effects
  ↪ M_2 model : capture more physical phenomena

Perspectives:

- Numerical scheme:
  ↪ higher order method
  ↪ convergence speed
  ↪ numerical diffusion
- More physics:
  ↪ pair production
  ↪ photoelectric effects
- Moment problem
  ↪ caracterizing realizability
  ↪ construct other closures
- Optimization

Thanks for your attention