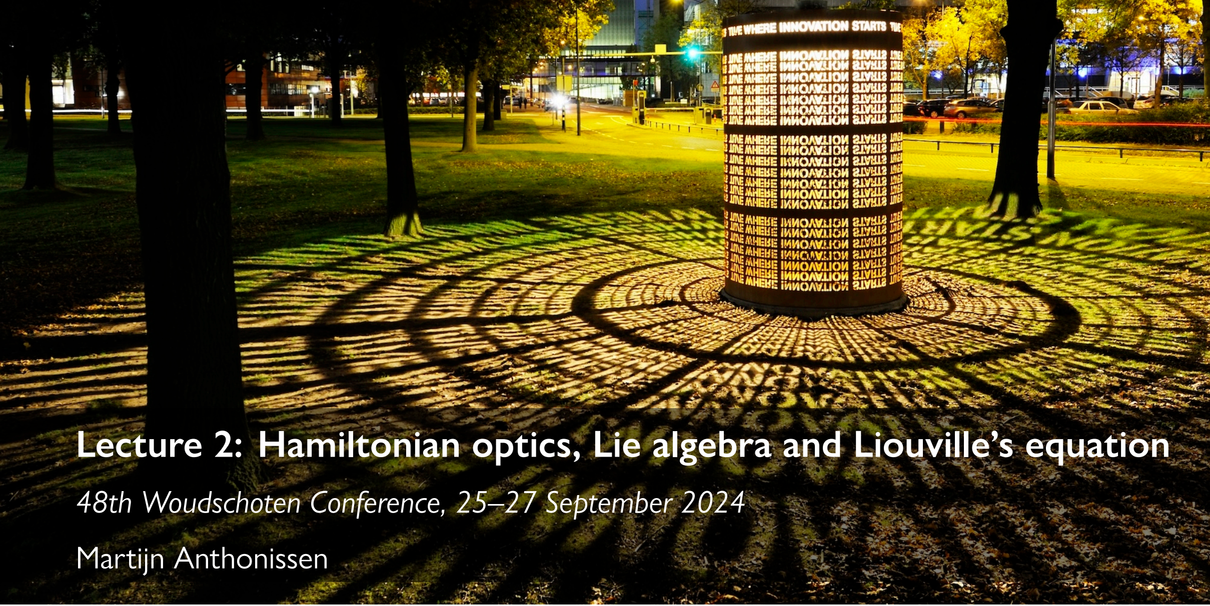


Lecture 2: Hamiltonian optics, Lie algebra and Liouville's equation

48th Woudschoten Conference, 25–27 September 2024

Martijn Anthonissen

Computational Illumination Optics Group

EINDHOVEN UNIVERSITY OF TECHNOLOGY

Outline

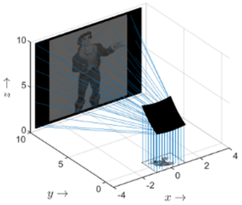
Computational illumination optics at TU/e

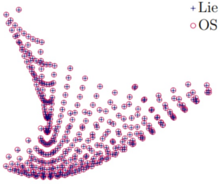
Hamiltonian optics

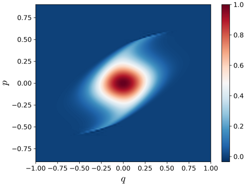
Imaging optics
- Aberrations
- Analytical expressions for aberrations
- Lie algebraic tools
- Numerical results

Improved direct methods
- Liouville's equation
- Discretization
- Numerical results

Conclusions







TU/e

Computational Illumination Optics Group at TU/e


Martijn Anthonissen


Wilbert IJzerman
Signify Research


Lisa Kusch

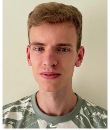

Koondi Mitra


Jan ten Thije Boonkkamp

OPTIC
AWAVE
Math & CS
OTP


Antonio Barion


Pieter Braam


Roel Hacking


Willem Jansen


René Köhle


Sanjana Verma


2024
Teun van Roosmalen

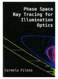

2024
Vì Kronberg


2023
Maikel Bertens


2023
Robert van Gestel

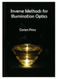

2021
Lotte Romijn


2018
Nitin Yadav



2018
Carmela Filosa

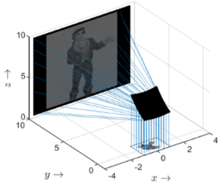

2017
Bart van Lith



2014
Corien Prins

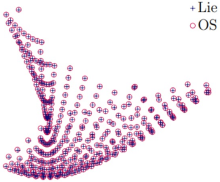
Lines of research

Line A
Nonimaging freeform optics



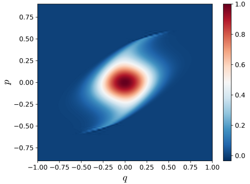
- Luminaires, street lights, …
- Compute optical surfaces that convert given source into desired target distribution
- Freeform surfaces
- Fully nonlinear PDE of Monge-Ampère type

Line B
Imaging optics



- Cameras, telescopes, …
- Make a very precise image of an object, minimizing aberrations
- Description with Lie transformations

Line C
Improved direct methods



- Ray tracing: iterative procedure to compute final design. Slow convergence
- Advanced numerical schemes for Hamiltonian systems and Liouville's equation

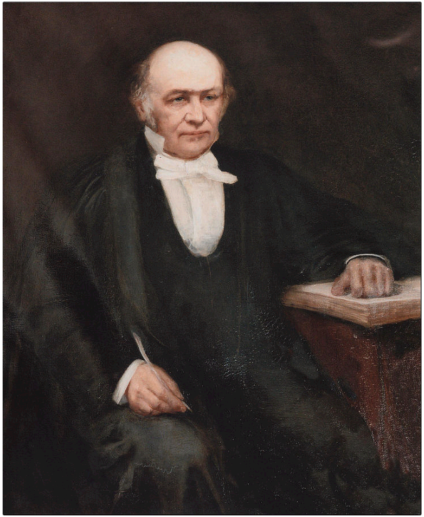
William Rowan Hamilton

Sir William Rowan Hamilton (1805–1865)

Irish mathematician, astronomer and physicist

Work

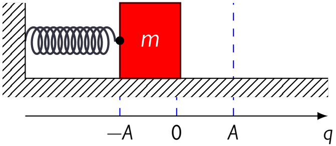
- Geometrical optics
- Classical mechanics
- Quaternions $i^2 = j^2 = k^2 = ijk = -1$



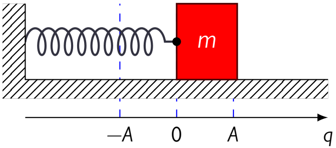
TU/e

Mass-spring system

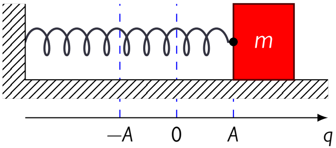
- Compressed spring



- Equilibrium position



- Extended spring



- Position of mass relative to equilibrium position: $q(t)$
- Momentum: $p(t) = mv(t) = m\dot{q}(t)$
- Hamiltonian:

$$H(q,p) = \frac{p^2}{2m} + \tfrac{1}{2}kq^2$$

- Hamilton's equations:

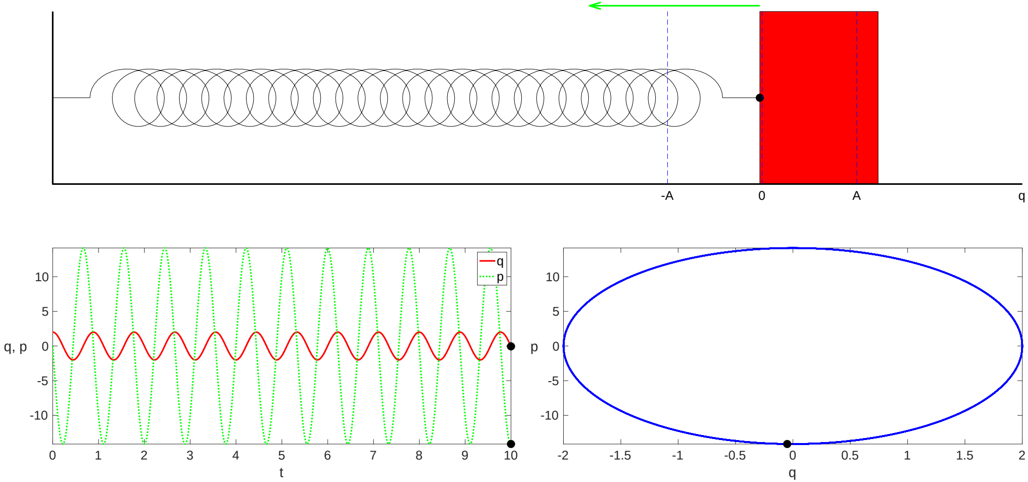
$$\dot{q} = \frac{\partial H}{\partial p}$$

$$\dot{p} = -\frac{\partial H}{\partial q}$$

- H is conserved:

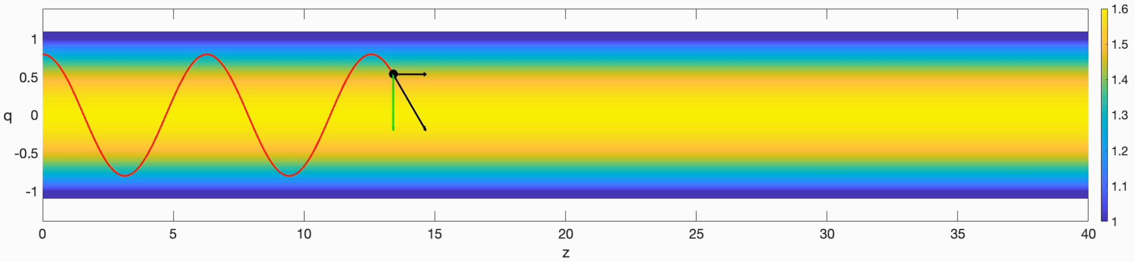
$$\dot{H} = \frac{\partial H}{\partial q}\dot{q} + \frac{\partial H}{\partial p}\dot{p} = 0$$

Simulation mass-spring system



This slide has an animation. It is available online at https://youtu.be/CE9GI80qQ0E

Optical fiber

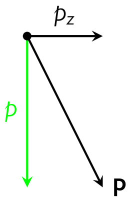


- Gradient-index material
  Refractive index $(-1 \leq q \leq 1)$

$$n(q) = \sqrt{n_0^2(1 - q^2) + q^2}$$

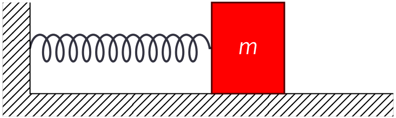
  Here: $n_0 > 1$
  Note: $1 \leq n(q) \leq n_0$
- Use z as evolution parameter

- Position: $q(z)$
- Optical momentum: $p(z) = n\dfrac{dq}{ds}$ with s arclength



$$\|\mathbf{p}\| = \sqrt{p^2 + p_z^2} = n$$

Hamiltonian system



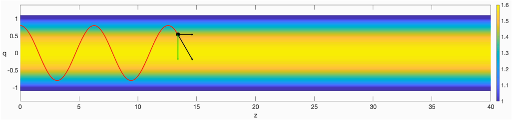
- Position of the mass: $q(t)$
- Momentum: $p(t)$
- Hamiltonian:

$$H(q,p) = \frac{p^2}{2m} + \tfrac{1}{2}kq^2$$

- Hamilton's equations:

$$\dot{q} = \frac{\partial H}{\partial p}$$

$$\dot{p} = -\frac{\partial H}{\partial q}$$



- Position of the ray: $q(z)$
- Optical momentum: $p(z)$
- Hamiltonian:

$$H(q,p) = -\sqrt{(n(q))^2 - p^2} = -p_z$$

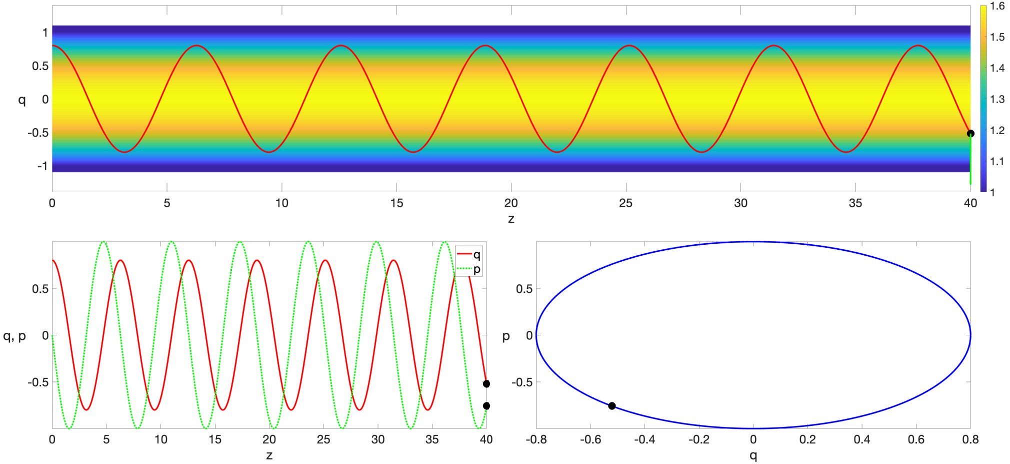
- Hamilton's equations:

$$\dot{q} = \frac{\partial H}{\partial p}$$

$$\dot{p} = -\frac{\partial H}{\partial q}$$

TU/e

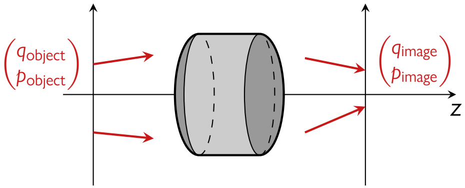
Simulation optical fiber



This slide has an animation. It is available online at https://youtu.be/exlVlEk8Ypk

Imaging optics

- Consider imaging optical system



- Each ray is defined by position $q(z)$ and optical momentum $p(z)$
- Hamiltonian optics:

$$\dot{q} = \frac{\partial H}{\partial p} \qquad \dot{p} = -\frac{\partial H}{\partial q} \qquad H = -\sqrt{n^2 - p^2}$$

- Optical map:

$$\begin{pmatrix} q_{\text{image}} \\ p_{\text{image}} \end{pmatrix} = M \begin{pmatrix} q_{\text{object}} \\ p_{\text{object}} \end{pmatrix}$$

Ideal system:

$$M = M_{\text{linear}} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

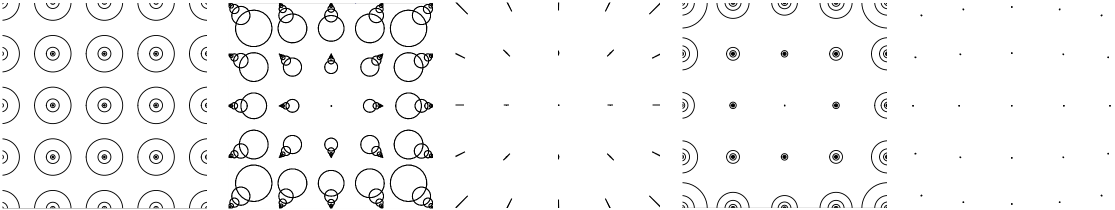
- In practice M is nonlinear
Goal: Mathematical description of deviations from linearity
- Deviations are called **aberrations** in optics

TU/e

Aberrations

- Consider Taylor series expansion of optical map in phase-space coordinates (q, p) about $(0, 0)$
- First-order term: Gaussian optics, paraxial optics
- Higher-order terms: aberrations
  Reducing aberrations is important for image quality
- Rotationally symmetric system: Odd-term aberrations only

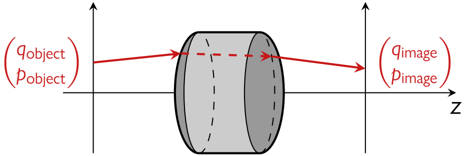
Third-order aberrations — image of regular 5×5 grid of point sources



Spherical aberration | Coma | Astigmatism | Field curvature | Distortion

Analytical expressions for aberrations

- **Goal:** Design optical systems with minimal aberrations
- **Needed:** Analytical expressions for aberrations
- Break down in steps: P—R—P—R—P P: propagation
  R: refraction



- Each step is symplectic map: No light rays lost or created
  Volume conservation in phase space
- Symplectic maps can be written as concatenation of *Lie transformations*

TU/e

Lie algebraic tools

- Let f, g, h be smooth functions on phase space
  Define **Poisson bracket** $[f, g]$

$$[f, g] = \frac{\partial f}{\partial q} \cdot \frac{\partial g}{\partial p} - \frac{\partial f}{\partial p} \cdot \frac{\partial g}{\partial q}$$

- Bi-linear

$$[\alpha f + \beta g, h] = \alpha [f, h] + \beta [g, h]$$
$$[f, \alpha g + \beta h] = \alpha [f, g] + \beta [f, h]$$

- Anti-commutative

$$[f, g] = -[g, f]$$

- Jacobi identity

$$[f, [g, h]] + [g, [h, f]] + [h, [f, g]] = 0$$

- Vector space of functions with Poisson bracket is **Lie algebra**
- Define **Lie operator** $[f, \cdot]$

$$[f, \cdot]g = [f, g]$$

- Define **Lie transformation** $\exp([f, \cdot])$

$$\exp([f, \cdot]) = \sum_{k=0}^{\infty} \frac{[f, \cdot]^k}{k!}$$
$$[f, \cdot]^0 = I$$
$$[f, \cdot]^k = [f, [f, \cdot]^{k-1}] \text{ for } k = 1, 2, \ldots$$

- Lie transformation is symplectic

Lie formulation of Hamiltonian optics

- Poisson bracket

$$[f, g] = \frac{\partial f}{\partial q} \cdot \frac{\partial g}{\partial p} - \frac{\partial f}{\partial p} \cdot \frac{\partial g}{\partial q}$$

- Note:

$$[H, q] = \frac{\partial H}{\partial q} \cdot \frac{\partial q}{\partial p} - \frac{\partial H}{\partial p} \cdot \frac{\partial q}{\partial q} = -\frac{\partial H}{\partial p}$$

$$[H, p] = \frac{\partial H}{\partial q} \cdot \frac{\partial p}{\partial p} - \frac{\partial H}{\partial p} \cdot \frac{\partial p}{\partial q} = \frac{\partial H}{\partial q}$$

- Recall Hamilton's equations:

$$\dot{q} = \frac{\partial H}{\partial p} \qquad \dot{p} = -\frac{\partial H}{\partial q}$$

- Rewrite as

$$\dot{q} = -[H, \cdot]q \qquad \dot{p} = -[H, \cdot]p$$

- It follows that

$$q^{(k)} = (-[H, \cdot])^k q$$

- Taylor series

$$q(z) = \sum_{k=0}^{\infty} \frac{q^k(0)}{k!} z^k$$

- Conclusion:

$$q(z) = M(q(0))$$
$$M = \exp(-z[H, \cdot])$$

TU/e

Propagation as Lie transformation

- Hamiltonian for light propagation in medium with constant refractive index n

$$H(q,p) = -\sqrt{n^2 - p^2}$$

- Taylor expansion:

$$H(q,p) = -n\sqrt{1-\left(\frac{p}{n}\right)^2} = -n + \frac{p^2}{2n} + \frac{p^4}{8n^3} + \cdots$$

- Lie transformation

$$\begin{aligned} M &= \exp(-z[H,\cdot]) \\ &= \exp(-z[-n,\cdot])\exp\left(\left[-z\frac{p^2}{2n},\cdot\right]\right)\exp\left(\left[-z\frac{p^4}{8n^3},\cdot\right]\right)\cdots \\ &= \exp(-z[H_2,\cdot])\exp(-z[H_4,\cdot])\cdots \end{aligned}$$

Barion, A., Anthonissen, M.J.H., ten Thije Boonkkamp, J.H.M., IJzerman, W.L. (2022)
Alternative computation of the Seidel aberration coefficients using the Lie algebraic method
Journal of the Optical Society of America A, Optics, Image Science and Vision, 39(9), 1603-1615
https://doi.org/10.1364/JOSAA.465900

Representing symplectic maps as Lie transformations

- **Dragt-Finn factorization**
  Let M be analytic symplectic map
  Assume $M(\mathbf{0}) = \mathbf{0}$
  Then:

  $$M = \exp([f_2, \cdot]) \exp([f_3, \cdot]) \exp([f_4, \cdot]) \cdots$$

  with f_m homogeneous polynomial of degree m:

  $$f_m(\lambda q, \lambda p) = \lambda^m f_m(q, p) \text{ for all } \lambda \in \mathbb{R}$$

- Approximate M by

  $$M \approx M_r = \exp([f_2, \cdot]) \exp([f_3, \cdot]) \cdots \exp([f_r, \cdot])$$

  Note: M_r is symplectic

- If g is homogeneous polynomial of degree m then

  $$[f_2, g] = \frac{\partial f_2}{\partial q} \cdot \frac{\partial g}{\partial p} - \frac{\partial f_2}{\partial p} \cdot \frac{\partial g}{\partial q}$$

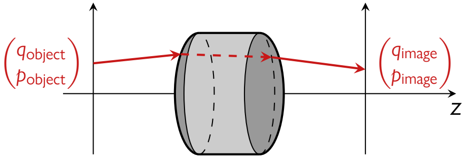
  has degree m too
  Same way: $[f_2, \cdot]^k g$ has degree m
  $\exp([f_2, \cdot])g$ has degree m
  $\exp([f_2, \cdot])$ is linear operator

- More general:
  $\exp([f_m, \cdot])$ describes aberrations of order $m - 1$

TU/e

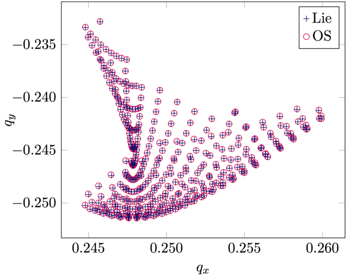
Analytical expressions for aberrations

- Consider imaging optical system



- Break down in steps: P—R—P—R—P
  P: propagation
  R: refraction
- Write each step as **truncated Lie transformation**
  Can be done for propagation, reflection, refraction
- Use the properties of Lie transformations to concatenate and rearrange them
- Use analytical expressions to design optical systems with minimal aberrations

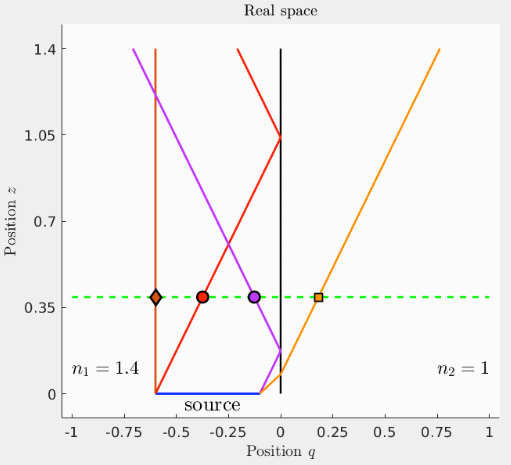
- Spot diagram off-axis object: Lie approach vs OpticStudio (OS)



Barion, A., Anthonissen, M.J.H., ten Thije Boonkkamp, J.H.M., IJzerman, W.L. (2023)
Computing aberration coefficients for plane-symmetric reflective systems: A Lie algebraic approach
Journal of the Optical Society of America A, Optics, Image Science and Vision, 40(6), 1215-1224
https://doi.org/10.1364/JOSAA.487343

TU/e

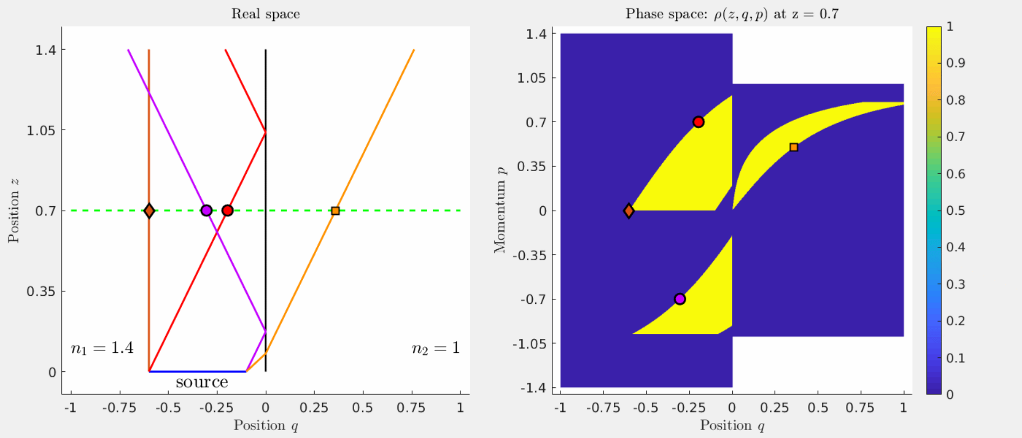
Improved direct methods based on solving Liouville's equation



- Direct method: given source and optical system, compute light distribution at target
- Standard: **Monte Carlo** ray tracing
  Robust but slow convergence (order $1/\sqrt{N_{\text{rays}}}$)
- Alternative: compute evolution of energy density in phase space by solving **Liouville's equation**
  Fast and more accurate
- $q < 0$: Water, refractive index $n_1 = 1.4$
  $q > 0$: Air, $n_2 = 1$
- Define ray by position $q(z)$ and direction $p(z)$
  ◆ $p(0) = 0 \longrightarrow q(z)$ constant
  ● $p(0) > p_{\text{crit}} \longrightarrow$ ray is reflected
  ● $p(0) > p_{\text{crit}} \longrightarrow$ ray is reflected
  ■ $0 < p(0) < p_{\text{crit}} \longrightarrow$ ray is refracted

TU/e

Phase space



This slide has an animation. It is available online at https://youtu.be/BRDN8DSwTNQ

TU/e

Liouville's equation

- Basic luminance $\rho = \rho(z, q, p)$: luminous flux per unit area and unit solid angle
- Along a ray:

$$\rho(z + \Delta z, q(z + \Delta z), p(z + \Delta z)) = \rho(z, q, p)$$

Differential form

$$\frac{\partial \rho}{\partial z} + \frac{\partial \rho}{\partial q}\dot{q} + \frac{\partial \rho}{\partial p}\dot{p} = 0$$

- Use Hamilton's equations

$$\dot{q} = \frac{\partial H}{\partial p} \qquad \dot{p} = -\frac{\partial H}{\partial q}$$

to get

$$\frac{\partial \rho}{\partial z} + \frac{\partial \rho}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial \rho}{\partial p}\frac{\partial H}{\partial q} = 0$$

- Liouville's equation

$$\frac{\partial \rho}{\partial z} + \nabla \cdot (\rho \mathbf{u}) = 0$$

with $\nabla = (\partial/\partial q, \partial/\partial p)^T$,

$$\mathbf{u} = \begin{pmatrix} \dfrac{\partial H}{\partial p} \\ -\dfrac{\partial H}{\partial q} \end{pmatrix}$$

- Using $H = -\sqrt{n^2 - p^2}$, we find

$$\mathbf{u} = \frac{1}{\sqrt{n^2 - p^2}} \begin{pmatrix} p \\ 0 \end{pmatrix}$$

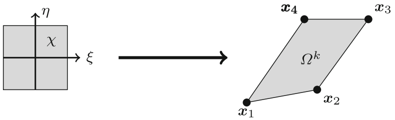
if n is constant. Hence:

$$\frac{\partial \rho}{\partial z} + u\frac{\partial \rho}{\partial q} = 0$$

TU/e

Space discretization

- 2D optical system: 2D phase space
  3D 4D
- Space discretization (q and p): **Discontinuous Galerkin spectral element method (DGSEM)**
- Straight-sided quadrilaterals



- Expand solution in reference domain $(\xi, \eta) \in [-1, 1]^2$

$$\rho(z, \xi, \eta) \approx \sum_{i=0}^{N} \sum_{j=0}^{N} \rho_{ij}(z) L_i(\xi) L_j(\eta)$$

  L_i, L_j: Lagrange polynomials on Gauss-Legendre nodes
- Accuracy controlled by number of elements K and polynomial order N
- Evolution of $\rho_{ij}(z)$ found from weak formulation of Liouville's equation

Optical interfaces

- At optical interfaces

$$\rho(z^-, q(z^-), p(z^-)) = \rho(z^+, q(z^+), p(z^+))$$

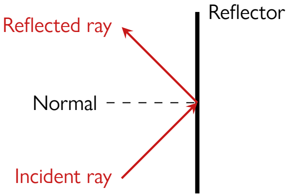
  z and q continuous
  p discontinuous

- Compute $p(z^+)$ from **law of reflection** or **Snell's law**

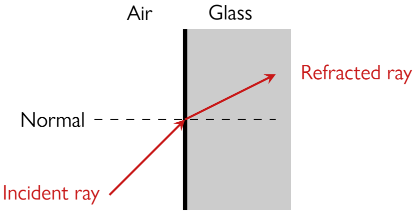
$$p(z^+) = S(p(z^-))$$

- Align mesh with optical interface
- Local energy balances to ensure energy conservation

- Reflection



- Refraction



TU/e

Time discretization

- Evolution parameter: z
  Arbitrary derivative (ADER) discretization
- Idea: use PDE to replace z-derivatives with spatial derivatives
- We have
$$\frac{\partial \rho}{\partial z} + u\frac{\partial \rho}{\partial q} = 0$$
  Taylor series:
$$\rho(z+\Delta z, q, p) \approx \sum_{k=0}^{M} \frac{1}{k!}\frac{\partial^k \rho}{\partial z^k}(z,q,p)(\Delta z)^k$$
  Replace z- with q-derivatives
$$\rho(z+\Delta z, q, p) \approx \sum_{k=0}^{M} C_k(\Delta z, q, p)\frac{\partial^k \rho}{\partial q^k}(z,q,p)$$
  Cauchy-Kovalewski procedure

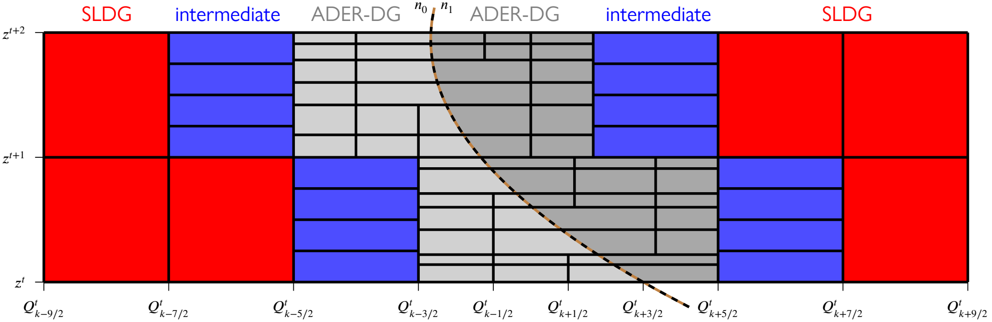
- ADER-DG leads to explicit scheme
- Arbitrarily high order of accuracy in space (q and p) and time (z)
- CFL condition on Δz causes problems near optical interfaces: **sub-cell interface method**

van Gestel, R.A.M., Anthonissen, M.J.H., ten Thije Boonkkamp, J.H.M., IJzerman, W.L. (2023)
An ADER discontinuous Galerkin method on moving meshes for Liouville's equation of geometrical optics
Journal of Computational Physics, 488, 112208
https://doi.org/10.1016/j.jcp.2023.112208

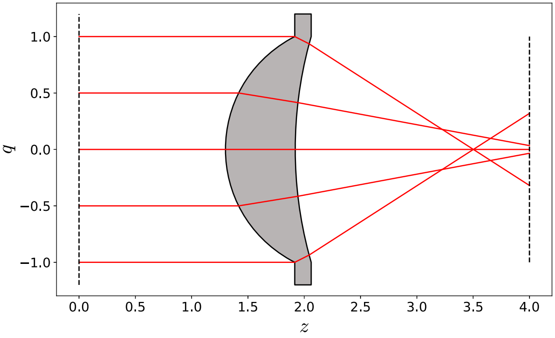
TU/e

Hybrid scheme

- Away from optical interfaces: light rays are straight lines if *n* is constant
- Can be solved more efficiently using **semi-Lagrangian discontinuous Galerkin (SLDG)** scheme
- Hybrid scheme: ADER-DG close to optical interface, SLDG elsewhere
- Divide computational domain in regions
  Intermediate element to couple ADER-DG and SLDG regions



Meniscus lens



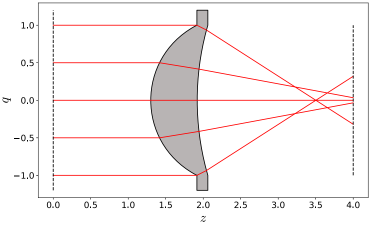
- Light rays travel from left to right
  Refracted at both spherical surfaces
- Initial condition ($z = 0$)

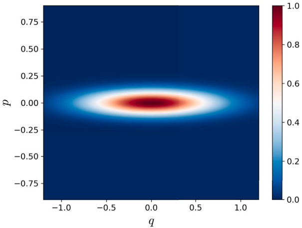
$$\rho(0, q, p) = \exp\left(\frac{-q^2}{2\sigma_q^2}\right) \exp\left(\frac{-p^2}{2\sigma_p^2}\right)$$

  with $\sigma_q = 0.5$, $\sigma_p = 0.08$
- Mesh: $\Delta q_{\max} = 0.16$, $\Delta p = 0.1$
  Polynomial order: $N = 7$

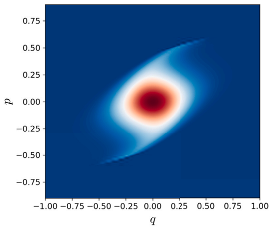
TU/e

Basic luminance

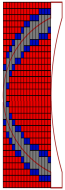




Initial condition



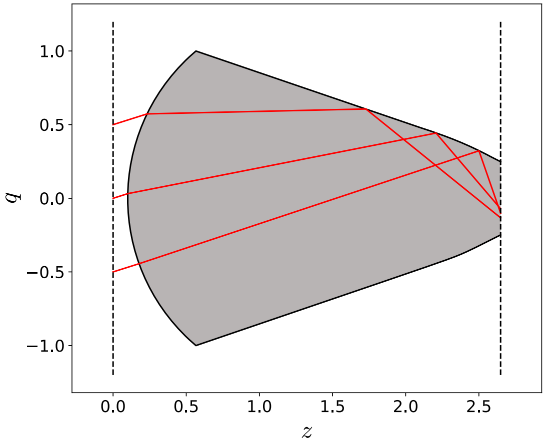
At target



van Gestel, R. A. M., Anthonissen, M. J. H.,
ten Thije Boonkkamp, J. H. M., IJzerman, W. L. (2024)
A hybrid semi-Lagrangian DG and ADER-DG solver on a moving mesh for Liouville's equation of geometrical optics
Journal of Computational Physics, 498, 112655
https://doi.org/10.1016/j.jcp.2023.112655

TU/e

Solar concentrator



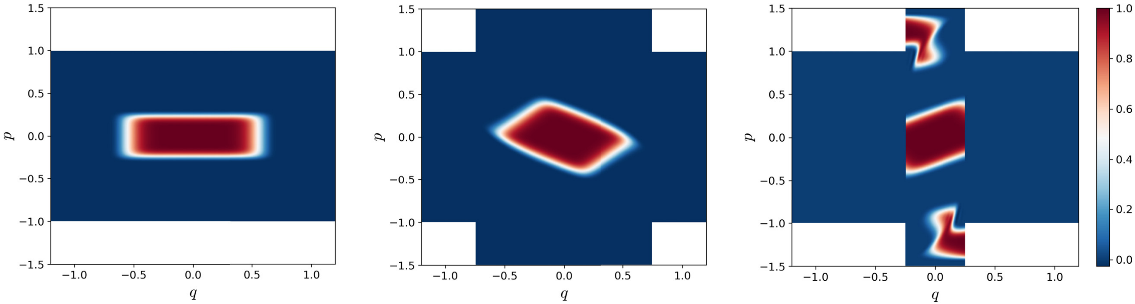
- Light rays travel from left to right
  Refracted at left surface
  Total internal reflection (TIR) at top or bottom
- ADER-DG scheme with initial condition ($z = 0$)

$$\rho(0, q, p) = \phi_{m,k}(q/\lambda_q)\phi_{m,k}(p/\lambda_p)$$

  with $\phi_{m,k}(x) = \cos^{m+1}\left(\frac{\pi}{2}x^k\right)$, $m = 10$, $k = 2$
- Mesh: $\Delta q_{\max} = 0.1$, $\Delta p = 0.1$
  Polynomial order: $N = 6$

TU/e

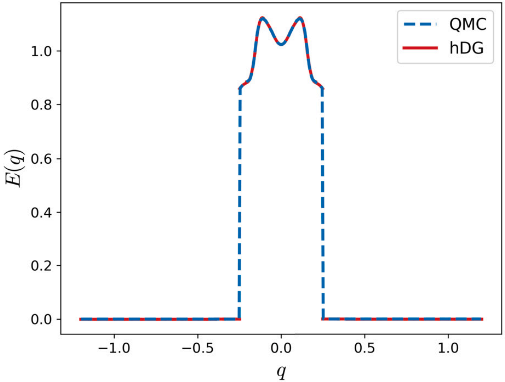
Basic luminance



Initial condition Half way At target

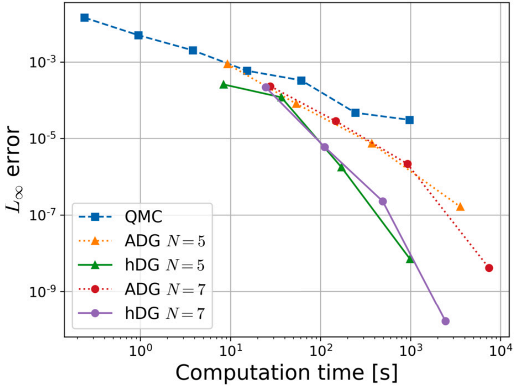
Animation at https://youtu.be/NdsmRIT2auE

Illuminance and comparison between methods



Illuminance at target

$$E(q) = \int \rho(z_{\text{target}}, q, p)\, dp$$

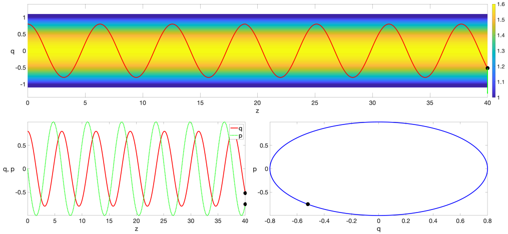


- QMC: quasi-Monte Carlo ray tracing
- ADG: ADER-DG
- hDG: hybrid scheme (ADER-DG and SLDG)

TU/e

Conclusions

- Model light propagation using Hamiltonian optics
- Nonlinearities in optical map: aberrations
  Reducing aberrations is important for image quality
- Approximate propagation, reflection and refraction
  by truncated Lie transformormations
- Concatenating and rearranging Lie transformations
  gives analytical expressions for aberrations
- Liouville's equation is alternative to ray tracing
- Advanced ADER-DG scheme to solve Liouville's equation
- Hybrid scheme: ADER-DG close to optical interface, SLDG elsewhere
  Outperforms ray tracing



OPTIC
AWAVE
Math & CS
OTP

More info: https://martijna.win.tue.nl/Optics/

TU/e