Computational High Frequency Wave Propagation

Olof Runborg

CSC, KTH

Isaac Newton Institute
Cambridge, February 2007
Outline

1. Introduction, background
2. Geometrical optics (GO)
3. Formulations of GO and numerical methods
   1. Eikonal equations
   2. Ray tracing
   3. Wavefront methods
   4. Kinetic formulation
   5. Phase space methods
4. Other models


Wave equation

- Cauchy problem for scalar wave equation

\[ u_{tt} - c(x)^2 \Delta u = 0, \quad (t, x) \in \mathbb{R}^+ \times \mathbb{R}^d, \]

\[ u(0, x) = A(x)e^{i\omega \phi(x)}, \quad u_t(0, x) = \omega B(x)e^{i\omega \phi(x)}, \]

where \( c(x) \) (variable) speed of propagation.

- Helmholtz equation \((u = v \exp(i\omega t))\)

\[ \Delta v + n(x)^2 \omega^2 v = f(x), \quad +\text{radiation condition}, \]

where \( n(x) := 1/c(x) \) index of refraction, \( \omega \) angular frequency.

- Scattering problem

- Similar versions for elastic wave equation, Maxwell equations, Schrödinger equation, . . . .
Computational challenge

- Simulation at high frequencies a major challenge!
  I.e., high relative to size of computational domain in time and space,

\[ \omega \gg \frac{1}{T}, \quad \frac{\omega}{c} = k \gg \frac{1}{X}. \]  
  (When \(0 \leq t \leq T\) and \(0 \leq x \leq X\).)
Simulation at high frequencies a major challenge!
I.e., high relative to size of computational domain in time and space,
\[ \omega \gg \frac{1}{T}, \quad \frac{\omega}{c} = k \gg \frac{1}{X}. \] (When \( 0 \leq t \leq T \) and \( 0 \leq x \leq X \).)

High frequency →
short wave length →
highly oscillatory solutions →
many gridpoints.
Computational challenge

- Simulation at high frequencies a major challenge!
  I.e., high relative to size of computational domain in time and space,

  \[ \omega \gg \frac{1}{T}, \quad \frac{\omega}{c} = k \gg \frac{1}{X}. \]
  (When \(0 \leq t \leq T\) and \(0 \leq x \leq X\).)

- High frequency → short wave length → highly oscillatory solutions → many gridpoints.

- Direct numerical solution resolves wavelength:
  \#gridpoints \sim \omega^d \text{ at least.}
Simulation at high frequencies a major challenge!
I.e., high relative to size of computational domain in time and space,

\[ \omega \gg \frac{1}{T}, \quad \frac{\omega}{c} = k \gg \frac{1}{X}. \]  

(When \( 0 \leq t \leq T \) and \( 0 \leq x \leq X \).

High frequency \( \rightarrow \) short wave length \( \rightarrow \) highly oscillatory solutions \( \rightarrow \) many gridpoints.

Direct numerical solution resolves wavelength:
\#gridpoints \( \sim \omega^d \) at least.

Often unrealistic approach for applications in e.g. optics, electromagnetics, geophysics, acoustics, ...
Challenge met by

- Efficient direct numerical methods
  (cost increases with $\omega$ for fixed accuracy)

- High frequency approximations
  (accuracy increases with $\omega$ for fixed cost)

- Prescribed tolerance methods for certain problems, [Bruno, Chandler-Wilde, ...]
  (cost independent of $\omega$ for fixed accuracy)
Geometrical optics

Helmholtz equation

\[ \Delta u + \omega^2 n(x)^2 u = 0. \]

Write solution on the form

\[ u(x) = A(x, \omega) e^{i \omega \phi(x)}. \]
Geometrical optics

Helmholtz equation

\[ \Delta u + \omega^2 n(x)^2 u = 0. \]

Write solution on the form

\[ u(x) = A(x, \omega) e^{i\omega \phi(x)}. \]

(a) Amplitude \( A(x) \)

(b) Phase \( \phi(x) \)

Solution \( u(x,y) \)
Geometrical optics

- Amplitude $A$ and phase $\phi$ vary on a much coarser scale than $u$. (And varies little with $\omega$.)
**Geometrical optics**

- Amplitude $A$ and phase $\phi$ vary on a much coarser scale than $u$. (And varies little with $\omega$.)
- Geometrical optics approximation considers $A$ and $\phi$ as $\omega \to \infty$.  

$$u(x) = A(x) e^{i \omega \phi(x)} + O\left(\frac{1}{\omega}\right).$$

⇒ Several amplitude and phase functions.
Amplitude $A$ and phase $\phi$ vary on a much coarser scale than $u$. (And varies little with $\omega$.)

Geometrical optics approximation considers $A$ and $\phi$ as $\omega \to \infty$.

Good accuracy for large $\omega$. Computational cost $\omega$-independent.

$$u(x) = A(x)e^{i\omega\phi(x)} + O(1/\omega).$$
Geometrical optics

- Amplitude $A$ and phase $\phi$ vary on a much coarser scale than $u$. (And varies little with $\omega$.)
- Geometrical optics approximation considers $A$ and $\phi$ as $\omega \to \infty$.
- Good accuracy for large $\omega$. Computational cost $\omega$-independent.

$$u(x) = A(x)e^{i\omega \phi(x)} + O(1/\omega).$$

- Waves propagate as rays, c.f. visible light. Not all wave effects captured correctly (diffraction, caustics).
Geometrical optics

- Amplitude $A$ and phase $\phi$ vary on a much coarser scale than $u$. (And varies little with $\omega$.)
- Geometrical optics approximation considers $A$ and $\phi$ as $\omega \to \infty$.
- Good accuracy for large $\omega$. Computational cost $\omega$-independent.

$$u(x) = A(x) e^{i\omega \phi(x)} + O(1/\omega).$$

- Waves propagate as rays, c.f. visible light. Not all wave effects captured correctly (diffraction, caustics).
- More generally, multiple crossing waves:

$$u(x) = \sum_{n=1}^{N} A_n(x) e^{i\omega \phi_n(x)} + O(1/\omega).$$

$\Rightarrow$ Several amplitude and phase functions.
GO approximation breaks down when the wavelength $\sim$ variations in $c(x)$. 
Limitations of geometrical optics

GO approximation breaks down when the wavelength $\sim$ variations in $c(x)$.

By the geometrical theory of diffraction (GTD) ([Keller, 59]) errors can be much larger than $O(1/\omega)$ because of boundaries:
- Diffracted waves
Limitations of geometrical optics

Diffracted waves
Limitations of geometrical optics

GO approximation breaks down when the wavelength $\sim$ variations in $c(x)$.

By the geometrical theory of diffraction (GTD) ([Keller, 59]) errors can be much larger than $O(1/\omega)$ because of boundaries:

- Diffracted waves
GO approximation breaks down when the wavelength $\sim$ variations in $c(x)$.

By the **geometrical theory of diffraction** (GTD) ([Keller, 59]) errors can be much larger than $O(1/\omega)$ because of boundaries:

- Diffracted waves
- Creeping rays
Limitations of geometrical optics

Creeping rays
Limitations of geometrical optics

GO approximation breaks down when the wavelength $\sim$ variations in $c(x)$.

By the geometrical theory of diffraction (GTD) ([Keller, 59]) errors can be much larger than $O(1/\omega)$ because of boundaries:

- Diffracted waves
- Creeping rays
Limitations of geometrical optics

GO approximation breaks down when the wavelength $\sim$ variations in $c(x)$.

By the geometrical theory of diffraction (GTD) ([Keller, 59]) errors can be much larger than $O(1/\omega)$ because of boundaries:

- Diffracted waves
- Creeping rays

Disappear in GO limit, but is of size $1/\omega^\alpha$, $0 < \alpha < 1$. (Hence $\gg 1/\omega$.)

GTD used in numerical simulations by e.g. adding diffracted waves at corners.
Limitations of geometrical optics

GO approximation breaks down when the wavelength $\sim$ variations in $c(x)$.

By the geometrical theory of diffraction (GTD) ([Keller, 59]) errors can be much larger than $O(1/\omega)$ because of boundaries:

- Diffracted waves
- Creeping rays

Disappear in GO limit, but is of size $1/\omega^\alpha$, $0 < \alpha < 1$. (Hence $\gg 1/\omega$.)

GTD used in numerical simulations by e.g. adding diffracted waves at corners.

Caustics is another problem: Amplitude $A$ infinite, but should be $A \sim \omega^\alpha$, $0 < \alpha < 1$. 
Limitations of geometrical optics

Caustics

Concentration of rays.

\[ A \to \infty \text{ when } \omega \to \infty. \]
GO approximation breaks down when the wavelength $\sim$ variations in $c(x)$.

By the geometrical theory of diffraction (GTD) ([Keller, 59]) errors can be much larger than $O(1/\omega)$ because of boundaries:
- Diffracted waves
- Creeping rays

Disappear in GO limit, but is of size $1/\omega^\alpha$, $0 < \alpha < 1$. (Hence $\gg 1/\omega$.)

GTD used in numerical simulations by e.g. adding diffracted waves at corners.

Caustics is another problem: Amplitude $A$ infinite, but should be $A \sim \omega^\alpha$, $0 < \alpha < 1$. 
Geometrical optics models and numerical methods

\[ \Delta u + \omega^2 n(x)^2 u = 0 \]

- **Rays**
  \[ \frac{dx}{dt} = c^2 p, \quad \frac{dp}{dt} = -\frac{\nabla c}{c} \]
  - Ray tracing

- **Kinetic**
  \[ f_t + c^2 p \cdot \nabla_x f - \frac{1}{c} \nabla c \cdot \nabla p f = 0 \]
  - Wavefront methods

- **Eikonal**
  \[ |\nabla \phi| = n(x) \]
  - Moment methods, Phase space methods

- **Hamilton–Jacobi methods**
Numerical and modeling issues

Goal:
Find phase (traveltime) and amplitude in a domain, on a regular grid.

Issues:
- Multiple arrivals, crossing rays, superposition multivaluedness.
- Eulerian/Lagrangian model. Fixed/moving grids. PDE/ODE model.
- Complexity.
Geometrical optics models and numerical methods

\[ \Delta u + \omega^2 n(x)^2 u = 0 \]

- Rays
  \[ \frac{dx}{dt} = c^2 p, \quad \frac{dp}{dt} = -\frac{\nabla c}{c} \]
  Ray tracing

- Kinetic
  \[ f_t + c^2 p \cdot \nabla_x f - \frac{1}{c} \nabla c \cdot \nabla_p f = 0 \]
  Wavefront methods

- Eikonal
  \[ |\nabla \phi| = n(x) \]
  Moment methods, Phase space methods

- Hamilton–Jacobi methods
Make the WKB ansatz

\[ u(x) = e^{i\omega \phi(x)} \sum_{k=0}^{\infty} a_k(x)(i\omega)^{-k}. \]
Eikonal- and transport equations

Derivation

Make the WKB ansatz

\[ u(x) = e^{i\omega \phi(x)} \sum_{k=0}^{\infty} a_k(x)(i\omega)^{-k}. \]

Enter this into Helmholtz equation \( \Delta u + \omega^2 n^2 u = 0 \),

\[ \omega^2 (n^2 - |\nabla \phi|^2) u + i\omega (2\nabla \phi \cdot \nabla a_0 + \Delta \phi a_0) e^{i\omega \phi(x)} + O(\omega^0) = 0. \]
Make the WKB ansatz

\[ u(x) = e^{i\omega \phi(x)} \sum_{k=0}^{\infty} a_k(x)(i\omega)^{-k}. \]

Enter this into Helmholtz equation \( \Delta u + \omega^2 n^2 u = 0 \),

\[ \omega^2 (n^2 - |\nabla \phi|^2) u + i\omega (2\nabla \phi \cdot \nabla a_0 + \Delta \phi a_0) e^{i\omega \phi(x)} + O(\omega^0) = 0. \]

Equate coefficients of powers of \( \omega \) to zero:
Eikonal- and transport equations

Derivation

Make the WKB ansatz

$$u(x) = e^{i\omega \phi(x)} \sum_{k=0}^{\infty} a_k(x)(i\omega)^{-k}.$$ 

Enter this into Helmholtz equation $\Delta u + \omega^2 n^2 u = 0,$

$$\omega^2 (n^2 - |\nabla \phi|^2) u + i\omega (2\nabla \phi \cdot \nabla a_0 + \Delta \phi a_0) e^{i\omega \phi(x)} + O(\omega^0) = 0.$$ 

Equate coefficients of powers of $\omega$ to zero:

- For $\omega^2$ we get the *eikonal equation*
  
  $$|\nabla \phi| = n(x),$$
Make the WKB ansatz

\[ u(x) = e^{i\omega \phi(x)} \sum_{k=0}^{\infty} a_k(x)(i\omega)^{-k}. \]

Enter this into Helmholtz equation \( \Delta u + \omega^2 n^2 u = 0 \),

\[ \omega^2(n^2 - |\nabla \phi|^2)u + i\omega(2\nabla \phi \cdot \nabla a_0 + \Delta \phi a_0)e^{i\omega \phi(x)} + O(\omega^0) = 0. \]

Equate coefficients of powers of \( \omega \) to zero:
- For \( \omega^2 \) we get the eikonal equation
  \[ |\nabla \phi| = n(x), \]
- For \( \omega^1 \) we get the transport equation
  \[ 2\nabla \phi \cdot \nabla a_0 + a_0 \Delta \phi = 0. \]
Make the WKB ansatz

\[ u(x) = e^{i\omega \phi(x)} \sum_{k=0}^{\infty} a_k(x)(i\omega)^{-k}. \]

Enter this into Helmholtz equation \( \Delta u + \omega^2 n^2 u = 0 \),

\[ \omega^2(n^2 - |\nabla \phi|^2)u + i\omega(2\nabla \phi \cdot \nabla a_0 + \Delta \phi a_0)e^{i\omega \phi(x)} + O(\omega^0) = 0. \]

Equate coefficients of powers of \( \omega \) to zero:

- For \( \omega^2 \) we get the eikonal equation
  \[ |\nabla \phi| = n(x), \]
- For \( \omega^1 \) we get the transport equation
  \[ 2\nabla \phi \cdot \nabla a_0 + a_0 \Delta \phi = 0. \]

Discard rest of terms in series \((\omega \to \infty)\). Let \( A = a_0 \).
Eikonal equation

Hamilton–Jacobi type nonlinear PDE. Can be solved efficiently on fixed Eulerian grids.
Eikonal equation

Hamilton–Jacobi type nonlinear PDE. Can be solved efficiently on fixed Eulerian grids.

- Stationary version.

\[ |\nabla \phi| = n(x). \]

Fast marching [Sethian, Tsitsiklis] or fast sweeping methods [Zhao, Tsai, et al].
Eikonal equation

Hamilton–Jacobi type nonlinear PDE. Can be solved efficiently on fixed Eulerian grids.

- Stationary version.
  \[ |\nabla \phi| = n(x). \]

  Fast marching [Sethian, Tsitsiklis] or fast sweeping methods [Zhao, Tsai, et al].

- Time-dependent version.
  Wave equation plus ansatz \( u(t, x) \approx A(t, x)e^{i\omega \varphi(t, x)} \) give
  \[ \varphi_t + n(x)^{-1}|\nabla \varphi| = 0. \]

  Upwind, high-resolution (ENO, WENO) finite difference methods [Osher, Shu, et al]
Eikonal equation

Hamilton–Jacobi type nonlinear PDE. Can be solved efficiently on fixed Eulerian grids.

- **Stationary version.**
  \[ |\nabla \phi| = n(x). \]

  Fast marching [Sethian, Tsitsiklis] or fast sweeping methods [Zhao, Tsai, et al].

- **Time-dependent version.**
  Wave equation plus ansatz \( u(t, x) \approx A(t, x)e^{i\omega \varphi(t,x)} \) give
  \[ \varphi_t + n(x)^{-1}|\nabla \varphi| = 0. \]

  Upwind, high-resolution (ENO, WENO) finite difference methods [Osher, Shu, et al]
  (Note, if IC and BC match, \( \varphi = \phi - t \).)
Eikonal equation:

$$|\nabla \phi| = n(x),$$
Eikonal equation:

\[ |\nabla \phi| = n(x), \]

- Ansatz only treats one wave. In general crossing waves

\[ u(x) \approx A_1(x)e^{i\omega \phi_1(x)} + A_2(x)e^{i\omega \phi_2(x)} + \ldots \]
Eikonal equation: 

\[ |\nabla \phi| = n(x), \]

- Ansatz only treats one wave. In general crossing waves 

\[ u(x) \approx A_1(x)e^{i\omega \phi_1(x)} + A_2(x)e^{i\omega \phi_2(x)} + \ldots \]

- Nonlinear equation, no superposition principle
Eikonal equation:

$$|\nabla \phi| = n(x),$$

- Ansatz only treats one wave. In general crossing waves

$$u(x) \approx A_1(x)e^{i\omega \phi_1(x)} + A_2(x)e^{i\omega \phi_2(x)} + \ldots$$

- Nonlinear equation, no superposition principle
- Viscosity solution, kinks
Eikonal equation:

\[ |\nabla \phi| = n(x), \]

- Ansatz only treats one wave. In general crossing waves
  
  \[ u(x) \approx A_1(x)e^{i\omega \phi_1(x)} + A_2(x)e^{i\omega \phi_2(x)} + \ldots \]

- Nonlinear equation, no superposition principle
- Viscosity solution, kinks
- First arrival property: \( \phi_{visc}(x) = \min_n \phi_n(x) \)
Eikonal equation
First arrival property

Note:
- $\phi \sim \text{traveltime of the wave}$
- $\phi(x) = \text{constant (level sets) represent wave fronts}$
Eikonal equation
Example
Geometrical optics models and numerical methods

\[ \Delta u + \omega^2 n(x)^2 u = 0 \]

**Rays**

\[
\frac{dx}{dt} = c^2 p, \quad \frac{dp}{dt} = -\frac{\nabla c}{c}
\]

- Ray tracing

**Kinetic**

\[
f_t + c^2 p \cdot \nabla_x f = 0
\]

- Wavefront methods

**Eikonal**

\[ |\nabla \phi| = n(x) \]

- Moment methods, Phase space methods

- Hamilton–Jacobi methods
Geometrical optics models and numerical methods

\[ \Delta u + \omega^2 n(x)^2 u = 0 \]

**Rays**

\[ \frac{dx}{dt} = c^2 p, \quad \frac{dp}{dt} = -\frac{\nabla c}{c} \]

Ray tracing

**Kinetic**

\[ f_t + c^2 p \cdot \nabla_x f \]

\[ -\frac{1}{c} \nabla c \cdot \nabla p f = 0 \]

Wavefront methods

Moment methods, Phase space methods

**Eikonal**

\[ |\nabla \phi| = n(x) \]

Hamilton–Jacobi methods

Olof Runborg (KTH)
Ray tracing

Rays are the (bi)characteristics \((x(t), p(t))\) of the eikonal equation, given by ODEs

\[
\frac{dx}{dt} = c(x)^2 p, \quad \frac{dp}{dt} = -\frac{\nabla c(x)}{c(x)},
\]

\(p(t)\) is local ray direction, "slowness" vector.
Ray tracing

Rays are the (bi)characteristics \((x(t), p(t))\) of the eikonal equation, given by ODEs

\[
\frac{dx}{dt} = c(x)^2 p, \quad \frac{dp}{dt} = -\nabla c(x),
\]

\(p(t)\) is local ray direction, "slowness" vector.

Ray tracing “method of characteristics” for eikonal equation.
Ray tracing

Rays are the (bi)characteristics \((\mathbf{x}(t), \mathbf{p}(t))\) of the eikonal equation, given by ODEs

\[
\frac{d\mathbf{x}}{dt} = c(\mathbf{x})^2 \mathbf{p}, \quad \frac{d\mathbf{p}}{dt} = -\nabla c(\mathbf{x}) \frac{c(\mathbf{x})}{c(\mathbf{x})},
\]

\(\mathbf{p}(t)\) is local ray direction, "slowness" vector.

Ray tracing "method of characteristics" for eikonal equation.

If valid at \(t = 0\), then for all \(t > 0\):

- \(\nabla \phi(\mathbf{x}(t)) = \mathbf{p}(t)\),  \((\text{local ray direction } \perp \text{ wavefronts})\)
Ray tracing

Rays are the (bi)characteristics \((x(t), p(t))\) of the eikonal equation, given by ODEs

\[
\frac{dx}{dt} = c(x)^2 p, \quad \frac{dp}{dt} = -\nabla c(x) / c(x),
\]

\(p(t)\) is local ray direction, "slowness" vector.

Ray tracing "method of characteristics" for eikonal equation.

If valid at \(t = 0\), then for all \(t > 0\):

- \(\nabla \phi(x(t)) = p(t)\), (local ray direction \(\perp\) wavefronts)
- \(\phi(x(t)) = t\), (phase \(\sim\) traveltime)
Ray tracing

Rays are the (bi)characteristics \( (x(t), p(t)) \) of the eikonal equation, given by ODEs

\[
\frac{dx}{dt} = c(x)^2 p, \quad \frac{dp}{dt} = -\nabla c(x) / c(x),
\]

\( p(t) \) is local ray direction, "slowness" vector.

Ray tracing “method of characteristics” for eikonal equation.

If valid at \( t = 0 \), then for all \( t > 0 \):

- \( \nabla \phi(x(t)) = p(t) \), (local ray direction \( \perp \) wavefronts)
- \( \phi(x(t)) = t \), (phase \( \sim \) traveltime)
- \( |p(t)| = 1 / c(x(t)) \), (can reduce to \( p \in S^{d-1} \), in 2D: \( p \sim \theta \))
Ray tracing

Rays are the (bi)characteristics \((x(t), p(t))\) of the eikonal equation, given by ODEs

\[
\frac{dx}{dt} = c(x)^2 p, \quad \frac{dp}{dt} = -\nabla c(x) c(x),
\]

\(p(t)\) is local ray direction, "slowness" vector.

Ray tracing “method of characteristics” for eikonal equation.

If valid at \(t = 0\), then for all \(t > 0\):

- \(\nabla \phi(x(t)) = p(t)\), (local ray direction \(\perp\) wavefronts)
- \(\phi(x(t)) = t\), (phase \(\sim\) traveltime)
- \(|p(t)| = 1/c(x(t))\), (can reduce to \(p \in S^{d-1}\), in 2D: \(p \sim \theta\))

There are also ODEs for the amplitude along rays.
Ray tracing
Numerics

Ray equations (with $|p| = 1/c$)

$$\frac{dx}{dt} = c(x)^2 p, \quad \frac{dp}{dt} = -\frac{\nabla c(x)}{c(x)},$$

Methods:

Standard numerical ODE methods, e.g. Runge Kutta.

If $c(x)$ is piecewise constant $\rightarrow$ rays piecewise straight lines refracted/reflected at interfaces by Snell's law.

(Geometrical problem, "shooting and bouncing rays" (SBR).)

Properties:

Rays can cross. (No problem with multivaluedness.)
Solution only given along rays. (Hard to interpolate traveltime to regular grid.)
Diverging rays. (Hard to cover full domain.)
Ray tracing
Numerics

Ray equations (with $|\mathbf{p}| = 1/c$)

$$\frac{dx}{dt} = c(x)^2 \mathbf{p}, \quad \frac{dp}{dt} = -\nabla c(x) / c(x),$$

Methods:
- Standard numerical ODE methods, e.g. Runge Kutta.
Ray equations (with $|\mathbf{p}| = 1/c$)

\[
\frac{d\mathbf{x}}{dt} = c(\mathbf{x})^2 \mathbf{p}, \quad \frac{d\mathbf{p}}{dt} = -\nabla c(\mathbf{x}) / c(\mathbf{x}),
\]

Methods:
- Standard numerical ODE methods, e.g. Runge Kutta.
- If $c(\mathbf{x})$ is piecewise constant $\rightarrow$
  rays piecewise straight lines refracted/reflected at interfaces by Snell’s law.
  (Geometrical problem, “shooting and bouncing rays” (SBR).)
Ray tracing
Numerics

Ray equations (with $|p| = 1/c$)

$$\frac{dx}{dt} = c(x)^2 p, \quad \frac{dp}{dt} = -\nabla c(x),$$

Methods:
- Standard numerical ODE methods, e.g. Runge Kutta.
- If $c(x)$ is piecewise constant $\rightarrow$
  rays piecewise straight lines refracted/reflected at interfaces by Snell’s law.
  (Geometrical problem, “shooting and bouncing rays” (SBR).)

Properties:
- Rays can cross. (No problem with multivaluedness.)
Ray equations (with $|p| = 1/c$)

\[
\frac{dx}{dt} = c(x)^2 p, \quad \frac{dp}{dt} = -\nabla c(x) / c(x),
\]

Methods:
- Standard numerical ODE methods, e.g. Runge Kutta.
- If $c(x)$ is piecewise constant $\rightarrow$ rays piecewise straight lines refracted/reflected at interfaces by Snell’s law. 
  (Geometrical problem, “shooting and bouncing rays” (SBR).)

Properties:
- Rays can cross. (No problem with multivaluedness.)
- Solution only given along rays. 
  (Hard to interpolate traveltime to regular grid.)
Ray equations (with $|p| = 1/c$)

\[
\frac{dx}{dt} = c(x)^2 p, \quad \frac{dp}{dt} = -\frac{\nabla c(x)}{c(x)},
\]

Methods:
- Standard numerical ODE methods, e.g. Runge Kutta.
- If $c(x)$ is piecewise constant → rays piecewise straight lines refracted/reflected at interfaces by Snell’s law.
  (Geometrical problem, “shooting and bouncing rays” (SBR).)

Properties:
- Rays can cross. (No problem with multivaluedness.)
- Solution only given along rays.
  (Hard to interpolate traveltime to regular grid.)
- Diverging rays. (Hard to cover full domain.)
Example: Ray tracing solution
Geometrical optics models and numerical methods

\[ \Delta u + \omega^2 n(x)^2 u = 0 \]

 Rays

\[ \frac{dx}{dt} = c^2 p, \quad \frac{dp}{dt} = -\frac{\nabla c}{c} \]

Ray tracing

Wavefront methods

Kinetic

\[ f_t + c^2 p \cdot \nabla_x f \]

\[-\frac{1}{c} \nabla c \cdot \nabla_p f = 0 \]

Moment methods, Phase space methods

Eikonal

\[ |\nabla \phi| = n(x) \]

Hamilton–Jacobi methods
Wavefronts

Wavefront given by \( \phi = \text{constant} \).
Suppose initial wavefront is \( \gamma(\alpha) \) and \( \phi(\gamma) = 0 \). Let

\[
x(t, \alpha), \quad p(t, \alpha)
\]

be the rays emitted orthogonal from this curve:

\[
x(0, \alpha) = \gamma(\alpha), \quad p(0, \alpha) = \frac{\gamma'(\alpha) \perp}{c|\gamma'(\alpha)|}.
\]

Wavefronts also given by: \( x(t = \text{constant}, \alpha) \). More general definition.

Introduce phase space \((x, p)\), where \(p \in \mathbb{S}^{d-1}\) is local ray direction.

Introduce phase space $(x, p)$, where $p \in S^{d-1}$ is local ray direction.

Observation: Wavefront is a smooth curve in phase space.

- 2D problems: 1D curve in 3D phase space $(x, y, \theta)$.
- 3D problems: 2D surface in 5D phase space $(x, y, z, \theta, \alpha)$. 

Olof Runborg (KTH)
Phase space


Introduce phase space $(x, p)$, where $p \in \mathbb{S}^{d-1}$ is local ray direction.

Observation: Wavefront is a smooth curve in phase space.
- 2D problems: 1D curve in 3D phase space $(x, y, \theta)$.
- 3D problems: 2D surface in 5D phase space $(x, y, z, \theta, \alpha)$.

Wavefront in phase space sweeps out a smooth surface – the Lagrangian submanifold.
Wavefront tracking

Directly solve for wavefront given by $x(t = \text{const}, \alpha)$. Suppose $\gamma(\alpha)$ is the initial wavefront, $x(0, \alpha) = \gamma(\alpha)$. Follow ensemble of rays

\[
\frac{\partial x(t, \alpha)}{\partial t} = c^2 p, \quad x(0, \alpha) = \gamma(\alpha),
\]

\[
\frac{\partial p(t, \alpha)}{\partial t} = -\nabla c, \quad p(0, \alpha) = \frac{\gamma'(\alpha) \perp}{c |\gamma'(\alpha)|}.
\]

Note: In principle we do not need to track $p$. Moving front in normal direction a possibility

\[
x_t = c \frac{x_{\perp}}{|x_{\alpha}|} \quad (\text{since } 0 = \partial_{\alpha} \phi(x(t, \alpha)) = x_{\alpha} \cdot \nabla \phi = x_{\alpha} \cdot p)
\]

But not good numerically since wavefront non-smooth!
Wavefront construction [Vinje, Iversen, Gjöystdal, Lambaré, ...]

- Solve for $\mathbf{x}(t, \alpha)$ and $p(t, \alpha)$. Discretize in $\alpha$ and trace rays for $\alpha_1, \alpha_2, \alpha_3, \ldots$ where $\alpha_j = j\Delta\alpha$.

$\mathbf{x}(t_n, \alpha_j)$
Wavefront construction [Vinje, Iversen, Gjøystdal, Lambaré, ...]

- Solve for $\mathbf{x}(t, \alpha)$ and $p(t, \alpha)$. Discretize in $\alpha$ and trace rays for $\alpha_1, \alpha_2, \alpha_3, \ldots$ where $\alpha_j = j \Delta \alpha$.
- Insert new rays adaptively by interpolation when front resolution deteriorates. E.g.:
  If $|\mathbf{x}(t_n, \alpha_{j+1}) - \mathbf{x}(t_n, \alpha_j)| \geq tol$ then insert new ray at $\alpha_{j+1}/2$.
Wavefront construction

- Solve for $x(t, \alpha)$ and $p(t, \alpha)$. Discretize in $\alpha$ and trace rays for $\alpha_1, \alpha_2, \alpha_3, \ldots$ where $\alpha_j = j \Delta \alpha$.

- Insert new rays adaptively by interpolation when front resolution deteriorates. E.g.:
  \[
  \text{If } |x(t_n, \alpha_{j+1}) - x(t_n, \alpha_j)| \geq tol \text{ then insert new ray at } \alpha_{j+1}/2.
  \]

- Interpolate traveltime/phase/amplitude onto regular grid.

\[x(t_n, \alpha_j)\]
Example: Wavefront tracking solution

- Multiple arrivals ok.
- Lagrangian method.
- Interpolation can be complicated.
Level set methods: Represent wavefront *implicitly* as the zero level set of a signed distance function $\phi(x)$.

\[ \gamma = \{ x \in \mathbb{R}^d : \phi(x) = 0 \}. \]
Wavefront in phase space higher co-dimension:
Represent as *intersection* of zero level sets of several functions. In 2D,
\[
\gamma = \{ \mathbf{x} \in \mathbb{R}^3 : \phi_1(\mathbf{x}) = 0, \phi_2(\mathbf{x}) = 0 \},
\]
\[
\phi_j = \phi_j(x, y, \theta).
\]

Level set functions satisfy linear hyperbolic PDEs:
\[
\partial_t \phi_j + c(x, y) \cos \theta \partial_x \phi_j + c(x, y) \sin \theta \partial_y \phi_j + (c_x \sin \theta - c_y \cos \theta) \partial_\theta \phi_j = 0.
\]

Use *local* level set method to reduce complexity.
Wavefront tracking, Eulerian versions
Segment projection method [Engquist, Tornberg, OR]

- Wavefront $\gamma$ is given as a union of curve segments $\gamma_j$.
- The segments are chosen such that they can be represented by a function of one coordinate variable: $f_i(t, x)$ and $g_j(t, y)$.
- From ray equations simple PDEs can be derived for $f_i$ and $g_j$. Ex: $\partial_t f_i + u \partial_x f_i = \nu$.
- Connectivity of segments is also maintained.

(a) Interface  
(b) $x$-segments  
(c) $y$-segments
Plane wave entering from the left.

(a) Local Ray Directions

(b) Wave Fronts
Segment projection method
Example, segments

\[
\begin{align*}
\text{x=0} & \quad \text{x=1} & \quad \text{x=2} \\
\sin(\theta) & \quad & \\
0 & \quad & \\
0.5 & \quad & \\
-0.5 & \quad & \\
0 & \quad & \\
1 & \quad & \\
2 & \quad & \\
y & \quad & \\
0 & \quad & \\
0.5 & \quad & \\
-0.5 & \quad & \\
0 & \quad & \\
1 & \quad & \\
2 & \quad & \\
\end{align*}
\]
Geometrical optics models and numerical methods

\[ \Delta u + \omega^2 n(x)^2 u = 0 \]

**Rays**

\[ \frac{dx}{dt} = c^2 p, \quad \frac{dp}{dt} = -\frac{\nabla c}{c} \]

- Ray tracing
- Wavefront methods

**Kinetic**

\[ f_t + c^2 p \cdot \nabla_x f - \frac{1}{c} \nabla c \cdot \nabla p f = 0 \]

- Moment methods
- Phase space methods

**Eikonal**

\[ |\nabla \phi| = n(x) \]

- Hamilton–Jacobi methods
Geometrical optics models and numerical methods

\[ \Delta u + \omega^2 n(x)^2 u = 0 \]

- Rays
  \[ \frac{dx}{dt} = c^2 p, \quad \frac{dp}{dt} = -\frac{\nabla c}{c} \]
  - Ray tracing
- Kinetic
  \[ f_t + c^2 p \cdot \nabla_x f - \frac{1}{c} \nabla c \cdot \nabla_p f = 0 \]
- Wavefront methods
- Moment methods, Phase space methods
- Eikonal
  \[ |\nabla \phi| = n(x) \]
- Hamilton–Jacobi methods

Olof Runborg (KTH)
High-Frequency Waves
INI, 2007
View rays as trajectories of particles. Let $f(t, x, p)$ be the particle (photon) density in phase space.
Kinetic formulation

- View rays as trajectories of particles. Let $f(t, x, p)$ be the particle (photon) density in phase space.
- Bicharacteristic equations $\Rightarrow$ Liouville equation

$$f_t + c^2 p \cdot \nabla_x f - \frac{\nabla c}{c} \cdot \nabla_p f = 0.$$
Kinetic formulation

- View rays as trajectories of particles. Let $f(t, x, p)$ be the particle (photon) density in phase space.

- Bicharacteristic equations $\Rightarrow$ Liouville equation

$$f_t + c^2 p \cdot \nabla_x f - \frac{\nabla c}{c} \cdot \nabla_p f = 0.$$ 

- A ray at $x$ in direction $p_0(t, x)$ and amplitude $A(t, x)$ represented as

$$f(t, x, p) = A^2(t, x) \delta(p - p_0(t, x)).$$
View rays as trajectories of particles. Let \( f(t, x, p) \) be the particle (photon) density in phase space.

Bicharacteristic equations \( \Rightarrow \) Liouville equation

\[
 f_t + c^2 p \cdot \nabla_x f - \frac{\nabla c}{c} \cdot \nabla p f = 0.
\]

A ray at \( x \) in direction \( p_0(t, x) \) and amplitude \( A(t, x) \) represented as

\[
 f(t, x, p) = A^2(t, x) \delta(p - p_0(t, x)).
\]

Since \( |p| = n(x) \), the density \( f \) supported on sphere \( |p| = n(x) \).
Liouville equation can also be derived directly from wave eq. through e.g. Wigner measures [Tartar, Lions, Paul, Gerard, Mauser, Markowich, Poupaud, ...]
Liouville equation can also be derived directly from wave eq. through e.g. Wigner measures [Tartar, Lions, Paul, Gerard, Mauser, Markowich, Poupaud, ...]

Let $f$ be limit of the Wigner transform of Helmholtz solution

$$
 f = \lim_{\omega \to \infty} F_{y\to p} u(x + y/2\omega) u(x - y/2\omega).
$$

Then $f$ satisfies Liouville eq.

$$
 f_t + c^2 p \cdot \nabla_x f - \frac{\nabla c}{c} \cdot \nabla_p f = 0.
$$
Kinetic formulation
Relation to Wigner theory

- Liouville equation can also be derived directly from wave eq. through e.g. Wigner measures [Tartar, Lions, Paul, Gerard, Mauser, Markowich, Poupaud, ...]

- Let $f$ be limit of the Wigner tranform of Helmholtz solution

\[
f = \lim_{\omega \to \infty} F_{y \to p} u(x + y/2\omega)u(x - y/2\omega).
\]

Then $f$ satisfies Liouville eq.

\[
f_t + c^2 p \cdot \nabla_x f - \frac{\nabla c}{c} \cdot \nabla p f = 0.
\]

- Relationship to wave equation solution:

\[
u = A e^{i\omega \phi} \sim f = A^2 \delta(p - \nabla \phi).
\]
Liouville equation can also be derived directly from wave eq. through e.g. Wigner measures [Tartar, Lions, Paul, Gerard, Mauser, Markowich, Poupaud, ...]

Let $f$ be limit of the Wigner transform of Helmholtz solution

$$f = \lim_{\omega \to \infty} F_{y \to p} u(x + y/2\omega)u(x - y/2\omega).$$

Then $f$ satisfies Liouville eq.

$$f_t + c^2 p \cdot \nabla_x f - \frac{\nabla c}{c} \cdot \nabla p f = 0.$$  

Relationship to wave equation solution:

$$u = Ae^{i\omega \phi} \sim f = A^2 \delta (p - \nabla \phi).$$

$$\lim_{\omega \to \infty} F_{y \to p} A(x + y/2\omega)A(x - y/2\omega)e^{i\omega(\phi(x+y/2\omega) - \phi(x-y/2\omega))}$$

$$= F_{y \to p} A^2(x)e^{iy \cdot \nabla \phi} = A^2 \delta (p - \nabla \phi).$$
Liouville equation can also be derived directly from wave eq. through e.g. Wigner measures [Tartar, Lions, Paul, Gerard, Mauser, Markowich, Poupaud, ...]

Let $f$ be limit of the Wigner transform of Helmholtz solution

$$f = \lim_{\omega \to \infty} \mathcal{F}_{y \to p} u(x + y/2\omega)u(x - y/2\omega).$$

Then $f$ satisfies Liouville eq.

$$f_t + c^2 p \cdot \nabla_x f - \frac{\nabla c}{c} \cdot \nabla_p f = 0.$$  

Relationship to wave equation solution:

$$u = Ae^{i\omega \phi} \sim f = A^2 \delta(p - \nabla \phi).$$

Note: Loss of phase information.
Moment equations

- Derived from Liouville equation in phase space + closure assumption for a system of equations representing the moments. (C.f. hydrodynamic limit from Boltzmann eq.)
Moment equations

- Derived from Liouville equation in phase space + closure assumption for a system of equations representing the moments. (C.f. hydrodynamic limit from Boltzmann eq.)
- Full equation for $f$ expensive to solve numerically. 6 independent variables in 3D.
Moment equations

- Derived from Liouville equation in phase space + closure assumption for a system of equations representing the moments. (C.f. hydrodynamic limit from Boltzmann eq.)
- Full equation for $f$ expensive to solve numerically. 6 independent variables in 3D.
- Moment eq is a PDE description in the “small” $(t, \mathbf{x})$-space. Fixed Eulerian grids can be used.
Moment equations

- Derived from Liouville equation in phase space + closure assumption for a system of equations representing the moments. (C.f. hydrodynamic limit from Boltzmann eq.)
- Full equation for $f$ expensive to solve numerically. 6 independent variables in 3D.
- Moment eq is a PDE description in the “small” $(t, x)$-space. Fixed Eulerian grids can be used.
- Arbitrary good superposition. $N$ crossing waves allowed. (But larger $N$ means a larger system of PDEs must be solved.)

[Brenier, Corrias, Engquist, OR] (wave equation),
[Gosse, Jin, Li, Markowich, Sparber] (Schrödinger)
Starting point is

\[ f_t + \mathbf{p} \cdot \nabla_x f = 0. \]

Let \( \mathbf{p} = (p_1, p_2) \). Define the moments,

\[ m_{ij} = \int_{\mathbb{R}^2} p_1^i p_2^j f \, d\mathbf{p}. \]

From

\[ \int_{\mathbb{R}^2} p_1^i p_2^j (f_t + \mathbf{p} \cdot \nabla_x f) \, d\mathbf{p} = 0, \]

we get the infinite (valid \( \forall i, j \geq 0 \)) system of moment equations

\[ (m_{ij})_t + (m_{i+1,j})_x + (m_{i,j+1})_y = 0. \]
Make the closure assumption

\[ f(x, p, t) = \sum_{k=1}^{N} A_k^2 \cdot \delta(p - p_k), \quad p_k = \begin{pmatrix} \cos \theta_k \\ \sin \theta_k \end{pmatrix}. \]

The moments take the form

\[ m_{ij} = \sum_{k=1}^{N} A_k^2 \cos^i \theta_k \sin^j \theta_k. \]

Corresponds to a maximum of \( N \) waves at each point.
Choose equations for moments \( m_{2k-1,0} \) and \( m_{0,2k-1} \), \( k = 1, \ldots, N \).
Gives closed system of \( 2N \) equations with \( 2N \) unknowns (the \( A_k \)'s and \( \theta_k \)'s).
Ex. $N = 1$

\[
\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}_t + \left( \frac{u_1^2}{\sqrt{u_1^2 + u_2^2}} \right) x + \left( \frac{u_1 u_2}{\sqrt{u_1^2 + u_2^2}} \right) y = 0.
\]

where $u_1 = m_{10} = A^2 \cos \theta$ and $u_2 = m_{01} = A^2 \sin \theta$.

For $N \geq 2$,

\[
F_0(u)_t + F_1(u)_x + F_2(u)_y = 0.
\]

where $F_0(u)$, $F_1(u)$ and $F_2(u)$ are complicated non-linear functions.

- PDE = weakly hyperbolic system of conservation laws, (with source terms when $c$ varies)
- Flux functions in conservation law can be difficult to evaluate.
Moment equations
Wedge example

(a) $N = 1$

(b) $N = 2$
Geometrical optics models and numerical methods

\[ \Delta u + \omega^2 n(x)^2 u = 0 \]

- Rays: 
  \[ \frac{dx}{dt} = c^2 p, \quad \frac{dp}{dt} = -\frac{\nabla c}{c} \]
  Ray tracing

- Kinetic: 
  \[ f_t + c^2 p \cdot \nabla_x f - \frac{1}{c} \nabla c \cdot \nabla_p f = 0 \]
  Wavefront methods

- Eikonal: 
  \[ |\nabla \phi| = n(x) \]
  Moment methods, Hamilton–Jacobi methods

Phase space methods
Eikonal solvers, wavefront tracking, etc. essentially constructed to solve the problem for one single initial data, e.g. a point source or a plane wave.

Solves for a "sheet" in phase space (the Lagrangian submanifold).

Some applications demand solution for many different sets of initial data (e.g. inverse problems).

Phase space methods: Get solution in the whole phase space. (Corresponds to solving for all possible initial data.)
Phase Space Methods, cont.

Equation to solve typically of the type time-independent Liouville equation/whole level set equation. (But other interpretation of unknown.)

- Computational cost:
  Suppose $N$ discretization points in each dimension.
  In 2D eikonal solvers/wavefront construction typically cost $O(N^2)$ for one initial data.
  Phase space methods cost $O(N^3 \log N)$ for all initial data.

- Combining advantages of using a fixed grid (cf eikonal solvers) and capturing multiple arrivals (cf ray methods) relatively easy.

- Examples: Phase Flow Method [Candès, Ying], Fast phase space method [Fomel, Sethian].
Integral formulation of scattering problem

$$u_s(x) = \int_{\partial \Omega} G(|x - x'|) \frac{\partial u(x')}{\partial n} dx', \quad x \in \mathbb{R}^d \setminus \Omega,$$

Approximate $\frac{\partial u}{\partial n}$ by geometrical optics solution. E.g. if $u_{inc} = \exp(i \omega \alpha \cdot x)$ is a plane wave, $\Omega$ convex, then

$$\frac{\partial u}{\partial n} \approx \frac{\partial (u_{inc} + u_{sGO})}{\partial n} = \begin{cases} 2i \omega \alpha \cdot \hat{n}(x)e^{i\omega\alpha \cdot x}, & x \text{ illuminated,} \\ 0, & x \text{ in shadow.} \end{cases}$$

Cost of evaluating solution still depends on $\omega$. 
For convex $\Omega$, make ansatz

$$\frac{\partial u}{\partial n} = i\omega A(x, \omega) e^{i\omega\alpha \cdot x}$$

then $A(x, \omega)$ smooth, uniformly in $\omega$, except at shadow boundaries. Discretize and solve $A(x, \omega)$ at cost independent of $\omega$. 

[Bruno, Chandler–Wilde, ...]
Complexity of simulation based on high-frequency approximations are not $\omega$-dependent.
Concluding remarks

- Complexity of simulation based on high-frequency approximations are not $\omega$-dependent.
- Error normally $O(1/\omega)$. Boundaries and caustic cause bigger errors. GTD reduces them.
Concluding remarks

- Complexity of simulation based on high-frequency approximations are not $\omega$-dependent.
- Error normally $O(1/\omega)$. Boundaries and caustic cause bigger errors. GTD reduces them.
- Trade-off point in $\omega$ increases with increasing computer power and is problem and accuracy dependent.
Concluding remarks

- Complexity of simulation based on high-frequency approximations are not $\omega$-dependent.

- Error normally $O(1/\omega)$. Boundaries and caustic cause bigger errors. GTD reduces them.

- Trade-off point in $\omega$ increases with increasing computer power and is problem and accuracy dependent.

- Challenges for geometrical optics methods include capturing multiple arrivals on fixed grids at reasonable complexity.
Concluding remarks

- Complexity of simulation based on high-frequency approximations are not $\omega$-dependent.
- Error normally $O(1/\omega)$. Boundaries and caustic cause bigger errors. GTD reduces them.
- Trade-off point in $\omega$ increases with increasing computer power and is problem and accuracy dependent.
- Challenges for geometrical optics methods include capturing multiple arrivals on fixed grids at reasonable complexity.
- Phase space methods useful when many similar problems need to be solved.
Concluding remarks

- Complexity of simulation based on high-frequency approximations are not $\omega$-dependent.
- Error normally $O(1/\omega)$. Boundaries and caustic cause bigger errors. GTD reduces them.
- Trade-off point in $\omega$ increases with increasing computer power and is problem and accuracy dependent.
- Challenges for geometrical optics methods include capturing multiple arrivals on fixed grids at reasonable complexity.
- Phase space methods useful when many similar problems need to be solved.
- Hybrid methods coupling elements of asymptotic models and direct methods a possibility.
Concluding remarks

- Complexity of simulation based on high-frequency approximations are not $\omega$-dependent.
- Error normally $O(1/\omega)$. Boundaries and caustic cause bigger errors. GTD reduces them.
- Trade-off point in $\omega$ increases with increasing computer power and is problem and accuracy dependent.
- Challenges for geometrical optics methods include capturing multiple arrivals on fixed grids at reasonable complexity.
- Phase space methods useful when many similar problems need to be solved.
- Hybrid methods coupling elements of asymptotic models and direct methods a possibility.
- Methods generalize to Maxwell, elastic wave eq, etc.
B. Engquist and O. Runborg.
Computational high-frequency wave propagation.

J.-D. Benamou.

O. Runborg.
Mathematical models and numerical methods for high frequency waves.