A Survey of Computational High Frequency Wave Propagation I

> Bjorn Engquist University of Texas at Austin

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Outline

- 1. Wave equations, scales and computational complexity
- 2. All frequency equations
- 3. Geometrical optics
- 4. High frequency approximations
- 5. Concluding remarks

1. Wave equations, scales and computational complexity

We will consider wave equations on the forms

- Scalar (\checkmark) $u_{tt} = c\Delta u$
- Elastic

 $\rho u_{tt} - \nabla \cdot \sigma(x, \nabla u) = 0$ $\begin{cases} \varepsilon E_t = \nabla \times H, & \nabla \cdot E = 0 \\ \mu H_t = -\nabla \times E, & \nabla \cdot H = 0 \end{cases}$ $(ih\psi_t + h^2 \Delta \psi = V\psi)$

- Maxwell
- (Schrödinger)

Computational challenge

A major challenge in simulations based on wave equations is computations at high frequencies. We mean here high frequencies relative to the size of the computational domain in space and time.

$$2\pi\omega >> T, \quad 0 \le t \le T$$
$$2\pi\omega/c = 2\pi k_x >> X, \quad 0 \le x \le X$$

high frequency \rightarrow short wave length \rightarrow highly oscillatory solution

The equations does not define the wave lengths or scales. They originate from geometry, initial and boundary conditions. (The same Maxwell's equations are valid from atomistic to galactic scales.)

The challenge are met by efficient numerical methods (c computational cost increases with increasing frequency ω) or by appropriate high frequency approximations (accuracy increases with increasing frequency ω).

Effective high frequency equations also give analytic insight (microlocal analysis) into the solution of wave equations, for example, propagation of singularities.

Computational complexity

- A major reason for deriving effective equations with a narrow range of scales in space and time is the high computational cost of directly solving multi-scale problems.
- Let the size of the computational domain = 1 in each dimension and the smallest wavelength=*ε*. The typical number of operations to achieve a prescribed accuracy in the solution of a multi-scale differential equation in d dimensions is,

 $flop = O((N(\varepsilon)\varepsilon^{-1})^{dr})$

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- $N(\varepsilon)$: number of unknowns per wavelength to achieve a given accuracy $(N(\varepsilon) \ge 2$ from Shannon sampling theorem, $N(\varepsilon) \approx O(\varepsilon^{-1/2})$ for standard second order finite difference methods).
- $\boldsymbol{\varepsilon}$: the shortest wavelength to be approximated
- d: number of dimensions
- *r:* exponent for number of flops per unknown in the numerical method (r=1 for explicit methods and r=3 for Gaussian elimination of dense matrices)

If r=1 and $N(\varepsilon)$ is bounded by a constant we have,

$$flop = O(\varepsilon^{-d})$$

Even with the best possible numerical methods $flop = O(\varepsilon^{-d})$, and this prohibits numerical simulation based on a full wave equation at high frequencies.

Note the limited role of adaptivity.

The upper limit for a teraflop computer is thus practically ε =10⁻⁴ with 10000 degrees of freedom in each dimension, *R*³⁺¹.

The number of wavelengths of light would be more than 10¹⁰ in dimensions of a typical room.



2. All frequency approximations

There are other types of approximations than the ones for high frequencies, which reduces the computational complexity. Examples are,

- Reduction in size of computational domain
- Reduction in number of independent variables
 - Frequency domain
 - Symmetries
- Reduced class of solutions
- Reductions based on simple c(x)
- Hybrid methods

All frequency approximations



Example of geometric approximations in the relative low frequency regime. Electro-magnetic field - wire interaction. Also example of Sub-grid scale modeling.

$$\mu \frac{\partial H}{\partial t} + \nabla \times E = 0 \qquad \qquad C \frac{\partial V}{\partial t} + \frac{\partial I}{\partial s} = 0$$
$$\varepsilon \frac{\partial E}{\partial t} - \nabla \times H = -\sigma E - \frac{I}{A} \delta_{\Gamma}(x) \qquad \qquad L \frac{\partial I}{\partial t} + \frac{\partial V}{\partial s} = E_s - RI$$



All frequency approximations



2. Geometrical optics

Geometrical optics equations are effective equations for high frequency wave propagation. Instead of directly approximating highly oscillatory functions geometrical optics gives the phase $\phi(x,t)$ and amplitude A(x,t).

In this case the effective formulation were known long before the wave equation form.

Note that new variables are introduced different from the strong or weak limit of the original dependent variables.



Scalar wave equation

$$\frac{\partial u^2(x,t)}{\partial t^2} = c(x)^2 \Delta u(x,t)$$
$$u(x,0) = u_0(x), \quad \frac{\partial u(x,0)}{\partial t} = u_1(x)$$

The velocity is denoted by *c* and the initial values are assumed to be highly oscillatory such that the following form is appropriate,

$$u(x,t) = \exp(i\omega\phi(x,t))\sum_{\omega=0}^{\infty} A_j(x,t)\omega^{-j}, \quad \omega >> 1$$

Insert the expansion into the wave equation and equate the different orders of ω (= ϵ^{-1}). The leading equations give the eikonal and transport equations that do not contain ω ,

$$\frac{\partial \phi}{\partial t} + c(x) |\nabla \phi| = 0, \quad (|\cdot| = Euclidean \ norm)$$
$$\frac{\partial A_0}{\partial t} + c(x) \frac{\nabla \phi \cdot \nabla A_0}{|\nabla \phi|} + \frac{c(x)^2 \Delta \phi - \frac{\partial^2 \phi}{\partial t^2}}{2c(x) |\nabla \phi|} A_0 = 0$$

The traditional ray tracing can be seen as the method of characteristics applied to the eikonal equation,



Remarks

- The analysis discussion above fails at boundaries. The geometrical theory of diffraction (GTD) adds correction terms for diffraction at corners and introduces the presence of creeping waves of the shadow zone.
- The approach extends to frequency domain formulations and other differential equations, for example, linear elasticity and Maxwell's equations.
- Compare WKB, Wigner transforms, path integrals and the Schrödinger equation.
- The nonlinear eikonal equation is of Hamilton Jacoby type and follows the viscosity solution theory.
- If c(x) = c(x,x/ε) is oscillatory, homogenization (ε << ω⁻¹), geometrical optics (ε >> ω⁻¹) or special expansions (ε ≈ ω⁻¹) apply.

4. High frequency approximations

The eikonal equation argument is the starting point for a wide class of formulations describing a wave equation solution for high frequencies. Compare semi classical approximations of quantum mechanics.

Some formulations are equivalent to the eikonal equations and some improves on geometrical optics.

high frequency approximations





high frequency approximations









high frequency approximations





5. Concluding remarks

Revisiting computational complexity

- $O(\omega^{4(1+1/p)})$, wave equation, time domain.
- $O(\omega^{3(1+1/p)r})$, wave equation, frequency domain, $1 \le 2 \le r \le 7/3$.
- O(ω^{2r}), boundary integral formulation (MoM), 1≤r ≤3 (from optimal iterative fast methods to direct methods).
- The complexity of simulation based on high frequency approximations are not ω dependent or improves with increasing ω .
- The trade off point in ω increases with increasing computing power and is problem and accuracy dependent.
- Note the possibility of hybridizing formulations