Numerical and asymptotic methods for highly oscillatory integrals

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8 October 2014, Woudschoten

Joint w. Sam Groth, Nele Lejon, Roel Matthysen, Peter Opsomer

Outline

1. An introduction to highly oscillatory problems
2. The wonderful world of asymptotic expansions
3. The numerical evaluation of oscillatory integrals

Outline

Definition

What is a *highly oscillatory problem*?

- a problem that involves highly oscillatory functions
- could be an ODE, PDE, integral equation, . . . or just an integral

When is a problem *highly oscillatory*?

- Say there is a typical wavelength λ and a typical size D in a problem
- then one looks at the ratio D/λ: how many wavelengths fit into the problem

Why are oscillatory problems hard?

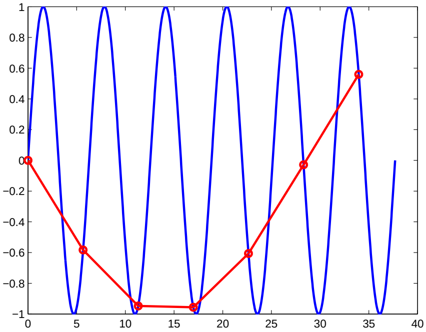
Three things make life difficult when oscillations increase:

1. Many degrees of freedom (dof) are required just to be able to represent the solution
   - 'resolving the oscillations'
2. Quite often, even more dof's are needed to solve a problem
   - due to pollution or dispersion errors[1]
3. Fast solvers for low-frequency problems typically fail (or need significant adjustments) for high-frequency problems
   - e.g. multigrid

[1] Babuska and Sauter, SIAM Review, 2000: Is the pollution effect of the FEM avoidable for the Helmholtz equation considering high wave numbers?

Sampling requirements

Use sufficiently many points, or this may happen:



Pollution errors

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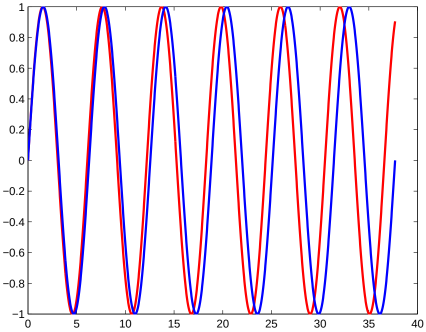

A crude computation

What is the computational cost of solving a highly oscillatory problem with frequency k?

1. Many degrees of freedom (dof) are required just to be able to represent the solution
   - fixed ndof's per wavelength and per dimension: $N = \mathcal{O}(k^d)$
2. Quite often, even more dof's are needed to solve a problem
   - pollution error: keep $k^2 h$ constant: $N = \mathcal{O}(k^{2d})$
3. Fast solvers for low-frequency problems typically fail for high-frequency problems
   - direct solver: cost is $\mathcal{O}(N^3) = \mathcal{O}(k^{6d})$

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A crude computation: example

What is the computational cost of solving a highly oscillatory problem with frequency k?

$$\mathcal{O}(k^{6d})$$

- When $d = 3$: cost scales as k^{18}.
- Clearly, we need to be more clever.

What can be done?

- Reduce pollution errors by using high-order methods:[2]
  - keep $k^{p+1}h^p$ constant: $N = \mathcal{O}(k^{2d}) \to N = \mathcal{O}(k^{d(1+1/p)})$
  - in other words: the number of points per wavelength does not have to grow like k
  - it is sufficient if it grows like $k^{1/p}$
- Remove pollution errors altogether by using integral equations
- Decrease dimension by using boundary integral equations: $N = \mathcal{O}(k^{d-1})$
- use fast solvers: Fast Multipole Methods are $\mathcal{O}(N \log N)$

Can we achieve a cost that is $\mathcal{O}(1)$?

[2] Bayliss, A., Goldstein, C.I., Turkel, E.: On accuracy conditions for the numerical computation of waves. J Comput Phys 1985

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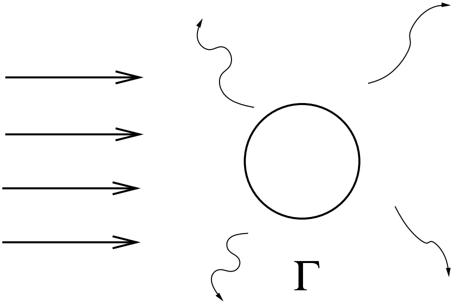
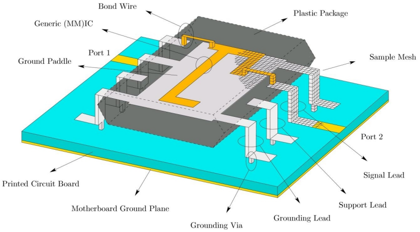
Boundary integral equations

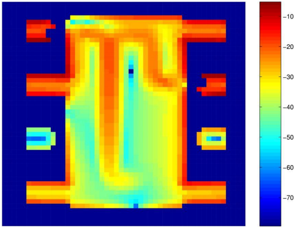
Where does the reduction in dimension come from:



We solve a problem defined on the boundary Γ of the scattering obstacle.

An example


Bond Wire
Plastic Package
Generic (MM)IC
Port 1
Ground Paddle
Sample Mesh
Port 2
Signal Lead
Printed Circuit Board
Support Lead
Motherboard Ground Plane
Grounding Lead
Grounding Via


−10
−20
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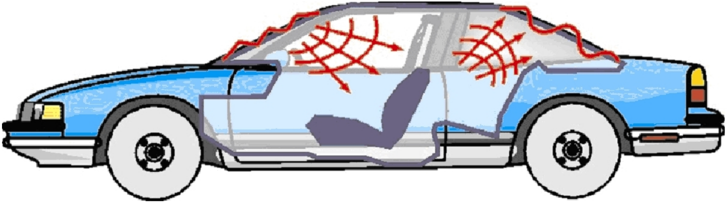
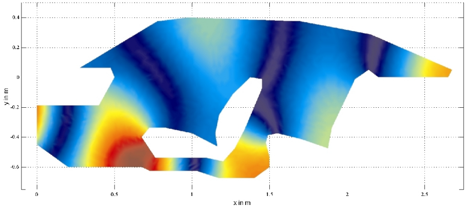
−50
−60
−70

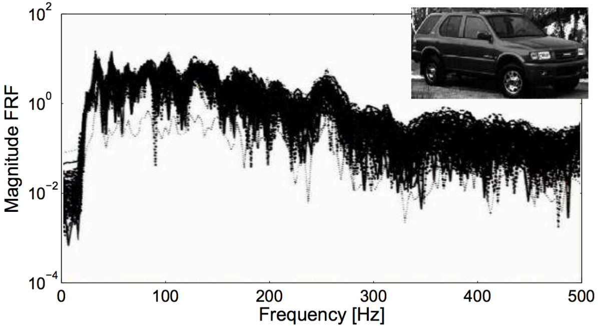
Another example





Should we solve highly oscillatory problems accurately?

Frequency response at driver's ear of 99 identical Isuzu Rodeo cars



Higher frequencies have larger variance in outcome.

Outline

1. An introduction to highly oscillatory problems
2. The wonderful world of asymptotic expansions
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We are off to a bad start . . .

There is a famous quote by Niels Henrik Abel (1802-1829):

> *"The divergent series are the invention of the devil, and it is a shame to base on them any demonstration whatsoever."*

This explains other statements, such as:

- J. P. Boyd, *The Devil's Invention: Asymptotic, Superasymptotic and Hyperasymptotic Series*, Acta Appl Math, 1999.
- $2 + 2 = 5$, for sufficiently large values of 2

The sentence that follows changes the picture

What Abel really said was:

> *"The divergent series are the invention of the devil, and it is a shame to base on them any demonstration whatsoever... Yet for the most part, the results are valid, it is true, but it is a curious thing. I am looking for the reason, a most interesting problem."*

Abel went on to describe Abel summation, a way of summing divergent series.

Two examples

- Asymptotics of orthogonal polynomials[3]
- Asymptotics of oscillatory integrals

[3] Opsomer et al, Construction and implementation of asymptotic expansions of Jacobi-type orthogonal polynomials, in preparation

The devil's invention

For large degree Legendre polynomials, we have (DLMF, 18.15.12)

$$P_n(\cos\theta) \sim \left(\frac{2}{\sin\theta}\right)^{1/2} \sum_{m=0}^{\infty} \binom{-\frac{1}{2}}{m} \binom{m-\frac{1}{2}}{n} \frac{\cos\alpha_{n,m}}{(2\sin\theta)^m}$$

but we also have[4]

$$\left(\frac{2}{\sin\theta}\right)^{1/2} \sum_{m=0}^{\infty} \binom{-\frac{1}{2}}{m} \binom{m-\frac{1}{2}}{n} \frac{\cos\alpha_{n,m}}{(2\sin\theta)^m} = \mathbf{2}P_n(\cos\theta)$$

So, what is the meaning of the first statement?

[4] FWJ Olver, A paradox in Asymptotics, SIAM J Math Anal 1(4), 1970

Accuracy of asymptotic expansions

If $f(n)$ has a *Poincaré-type* asymptotic expansion

$$f(n) \sim \sum_{k=1}^{\infty} a_k n^{-k}, \qquad n \gg 1$$

this means that

$$f(n) - \sum_{k=1}^{K} a_k n^{-k} = \mathcal{O}(n^{-K-1})$$

There is no convergence for fixed n, only convergence for increasing n.
Asymptotic expansions typically diverge.
There is no error control.

Accuracy of asymptotic expansions (2)

$$f(n) \sim \sum_{k=1}^{\infty} a_k n^{-k}, \qquad n \gg 1$$

Observations:

- The *optimal truncation point* is typically linear in n
- The *best achievable error* is typically exponentially small in n
- !Numerical computation of a_k is often numerically unstable!

There are still no guarantees for any fixed n. Clearly, we have to be more clever.

Design goal of hybrid numerical-asymptotic methods

Say $f(n)$ is the solution to $Lf = 0$. Say $Q[f]$ is the numerical solution to the approximate equation $L_h f = 0$. Then if

$$f(n) \sim \sum_{k=1}^{\infty} a_k n^{-k}, \qquad n \gg 1$$

and

$$g(n) \sim \sum_{k=1}^{\infty} b_k n^{-k}, \qquad n \gg 1$$

we want to make sure that $a_k = b_k$, $k = 1, \ldots, K$. In that case:

$$f(n) - g(n) = \mathcal{O}(n^{-K-1})$$

Outline

A model integral

A Fourier-type oscillatory integral has the form

$$I[f] = \int_a^b f(x) e^{i\omega g(x)} \mathrm{d}x$$

with

- f a non-oscillatory *envelope* or *amplitude* function
- g a non-oscillatory *phase* function
- $\omega \in \mathbb{R}$ a frequency parameter, potentially large

There are many variants. The case $g(x) = x$ is special.

How to derive an asymptotic expansion, part I

If all else fails, integrate by parts

Assume $g(x) = x$. Then

$$
\begin{aligned}
I[f] &= \int_a^b f(x) e^{i\omega x} \mathrm{d}x \\
&= \int_a^b f(x) \frac{1}{i\omega} \left(e^{i\omega x}\right)' \mathrm{d}x \\
&= \frac{1}{i\omega} f(x) e^{i\omega x} \Big|_a^b - \frac{1}{i\omega} \int_a^b f'(x) e^{i\omega x} \mathrm{d}x \\
&= \frac{1}{i\omega} \left[f(b) e^{i\omega b} - f(a) e^{i\omega a} \right] - \frac{1}{i\omega} \int_a^b f'(x) e^{i\omega x} \mathrm{d}x
\end{aligned}
$$

How large is $I[f]$ for large ω? It is $\mathcal{O}(\omega^{-1})$.

How to derive an asymptotic expansion, part I

Rinse, repeat:

$$\begin{aligned} I[f] &= \frac{1}{i\omega}\left[f(b)e^{i\omega b} - f(a)e^{i\omega a}\right] - \frac{1}{i\omega}\int_a^b f'(x)e^{i\omega x}\mathrm{d}x \\ &= \frac{1}{i\omega}\left[f(b)e^{i\omega b} - f(a)e^{i\omega a}\right] - \frac{1}{(i\omega)^2}\left[f'(b)e^{i\omega b} - f'(a)e^{i\omega a}\right] \\ &\qquad + \frac{1}{(i\omega)^2}\int_a^b f''(x)e^{i\omega x}\mathrm{d}x \\ &\sim \sum_{k=0}^{\infty} \frac{1}{(i\omega)^{k+1}}\left[f^{(k)}(b)e^{i\omega b} - f^{(k)}(a)e^{i\omega a}\right]. \end{aligned}$$

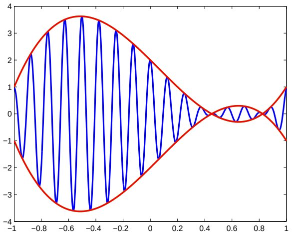
A simple numerical scheme: Filon quadrature

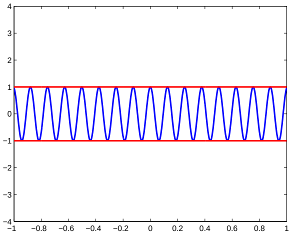
Approximate $I[f]$ by the exact integral $I[p]$ where p is a polynomial

- *Classical*: If $p \approx f$ then $I[f] - I[p] = I[f-p]$ is probably small
- *Asymptotic*: What if just $p(a) = f(a)$ and $p(b) = f(b)$?
  In that case:

$$I[f] - I[p] = \mathcal{O}(\omega^{-2})$$

$$f(x) = 5x^3 - x^2 - 5x + 2 \qquad\qquad p(x) = 1$$





Filon quadrature

Higher asymptotic convergence:[5]

$$p^{(k)}(a) = f^{(k)}(a) \qquad \text{and} \qquad p^{(k)}(a) = f^{(k)}(a), \qquad k = 0, \ldots, K-1$$

There are two driving forces for convergence

- *Classical*: making p approximate f better
- *Asymptotic*: making p agree with (derivatives of) f at the endpoints

How to combine the two optimally is an open problem!

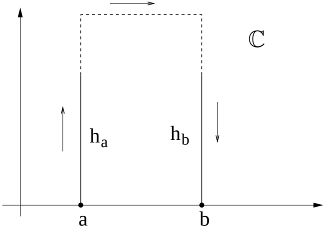
- Optimal points lie almost certainly in the complex plane.[6]

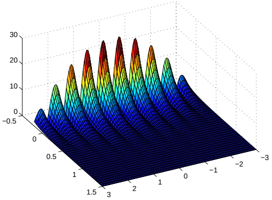
[5] Iserles and Norsett, 2005

[6] Asheim, Deano, H., Wang, 2013

How to derive an asymptotic expansion, part II

Let us deform the path of integration into the complex plane





$$
\begin{aligned}
I[f] &= \int_a^b f(x) e^{i\omega x} \mathrm{d}x \\
&= (?) \int_{h_a} f(z) e^{i\omega z} \mathrm{d}z - \int_{h_b} f(z) e^{i\omega z} \mathrm{d}z \\
&= e^{i\omega a} \int_0^\infty f(a+ip) e^{-\omega p} \mathrm{d}p - e^{i\omega b} \int_0^\infty f(b+ip) e^{-\omega p} \mathrm{d}p
\end{aligned}
$$

How to derive an asymptotic expansion, part II

We have ourselves a Laplace-type integral:

$$L[f] = \int_0^\infty f(p) e^{-\omega p} \mathrm{d}p$$

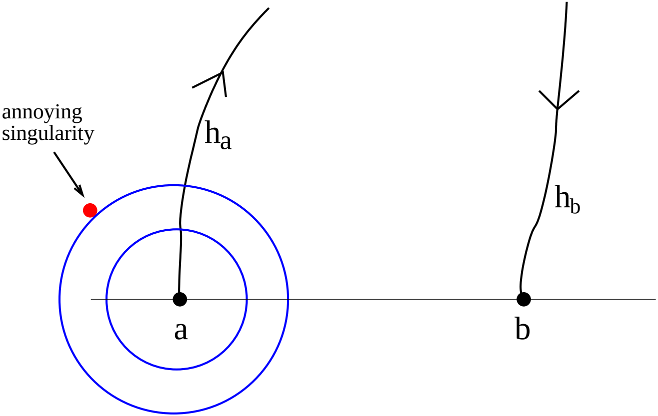
- localization near $p = 0$ from exponential decay of the integrand, more pronounced for large ω
- idea: replace f by its Taylor series at $p = 0$:

$$L[f] \sim \int_0^\infty \sum_{k=0}^\infty f^{(k)}(0) \frac{p^k}{k!} e^{-\omega p} \mathrm{d}p \sim \sum_{k=0}^\infty \frac{1}{\omega^{k+1}} f^{(k)}(0)$$

- **Watson's Lemma**: an asymptotic crime!

The root cause of divergence

We integrate the Taylor series of f outside its radius of convergence:



A second numerical method

Replacing f by a Taylor series is a bad idea. Let's use a different polynomial:

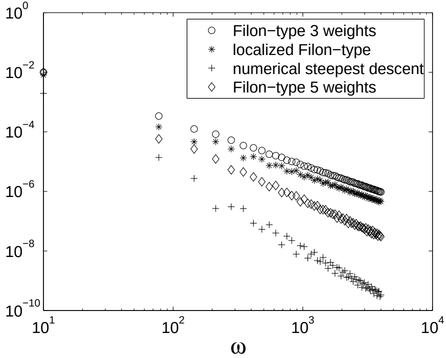
$$L[f] = \int_0^\infty f(p) e^{-\omega p} \mathrm{d}p = \frac{1}{\omega} \int_0^\infty f(q/\omega) e^{-q} \mathrm{d}q$$

- Use Gauss-Laguerre quadrature, with weight function e^{-q}. [7]
- Error behaves as ω^{-2K-1} using just K points
- Under certain conditions, convergence to $L[f]$

[7] H. and Vandewalle, On the efficient numerical evaluation of oscillatory integrals by analytic continuation, SIAM J Numer Anal, 2006.

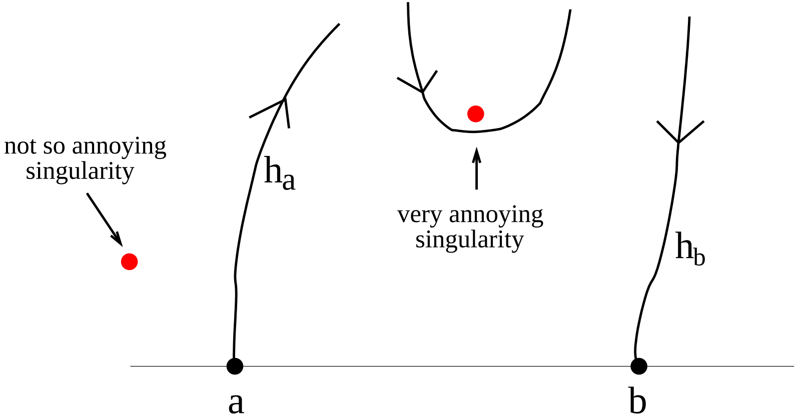
A small comparison

Typical convergence characteristics



Comparison of some methods that use between 3 and 5 evaluations of f.

Did we fix divergence? No!



The numerical method of steepest descent may in some cases not converge to $I[f]$. Also, the limit $\omega \to 0$ is not stable.

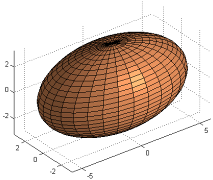
Further observations

- Issue with stationary points: $g'(\xi) = 0$ for g in $e^{i\omega g(x)}$
  - integration by parts: division by zero
  - path deformation: h_a and h_b do not connect at infinity
- Multiple coalescing stationary points: Nele Lejon
- Why points of reflection of rays scattered by obstacles correspond to stationary points of oscillatory integrals: Sam Groth

Example: a three-dimensional integral

An ellipsoid

$$I_3 := \int_E \frac{1}{4\pi} k^2 (n(\mathbf{x})^2 - 1) e^{i\omega\, \mathbf{a}\cdot\mathbf{x}}\, dx_3\, dx_2\, dx_1.$$



- length scales R_1, R_2, R_3 along X, Y and Z axis
- oscillator: $\mathbf{a}\cdot\mathbf{x} = a_1x_1 + a_2x_2 + a_3x_3$
- two resonance points
- application: scattering of light due to propagation in an object with refractive index $n(\mathbf{x})$ (S Trattner)

The end

Thanks!