Time domain / volume discretisation

1. Discretisation schemes
2. Explicit, implicit, and stability
3. Numerical Accuracy
4. Sources and boundary conditions
5. Perfectly absorbing layers
6. Handling additional terms in the equation
7. Grid refinement and subgridscale models
8. Implementation aspects

1. Discretisation schemes

a) Cartesian grids, collocated and staggered
b) Extended stencils
c) Non-Cartesian structured grids
d) Non-structured grids

1.a) Cartesian grids

- Collocated grids = all field variables discretised at same location (*i*,*j*,*k*) -> *x*=*i dx*, *y*=*j dy*, *z*=*k dz*
  - Popular in for example CFD (computational fluid dynamics)
  - Consider the spatial derivatives in

$$\frac{\partial \mathbf{o}}{\partial t} + \nabla p = 0 \qquad \frac{\partial p}{\partial t} + c^2 \nabla \cdot \mathbf{o} = 0$$

  - Without loss of generality, we can limit the discussion to one dimension (*x*)
  - Expand around (*i*,*j*,*k*), x_0=*i dx,* in the x direction

$$p(x_0 + dx) = p(x_0) + \frac{dx}{1!}\frac{\partial p}{\partial x}\bigg|_{x_0} + \frac{dx^2}{2!}\frac{\partial^2 p}{\partial x^2}\bigg|_{x_0} + \frac{dx^3}{3!}\frac{\partial^3 p}{\partial x^3}\bigg|_{x_0} + \dots$$

$$p(x_0 - dx) = p(x_0) - \frac{dx}{1!}\frac{\partial p}{\partial x}\bigg|_{x_0} + \frac{dx^2}{2!}\frac{\partial^2 p}{\partial x^2}\bigg|_{x_0} - \frac{dx^3}{3!}\frac{\partial^3 p}{\partial x^3}\bigg|_{x_0} + \dots$$

1.a) Cartesian grids

- Collocated (continued)
  - Subtracting gives

$$\left.\frac{\partial p}{\partial x}\right|_{x_0} = \frac{1}{2dx}\left(p(x_0+dx) - p(x_0-dx)\right) + \cancel{\left.\frac{dx^2}{3!}\frac{\partial^3 p}{\partial x^3}\right|_{x_0}} + \ldots$$

  - In this central differences approach, the second order derivative and corresponding first order dependence on *dx* drops out.
  - This scheme is second order accurate.

  - The spatial derivative at x_0 only depends on values in the next and previous cell.
  - It is easy to see that odd index *p* only depend on even index **o** values and vice versa.
  - Small spatial changes in sources or structure cause problems.

1.a) Cartesian grids

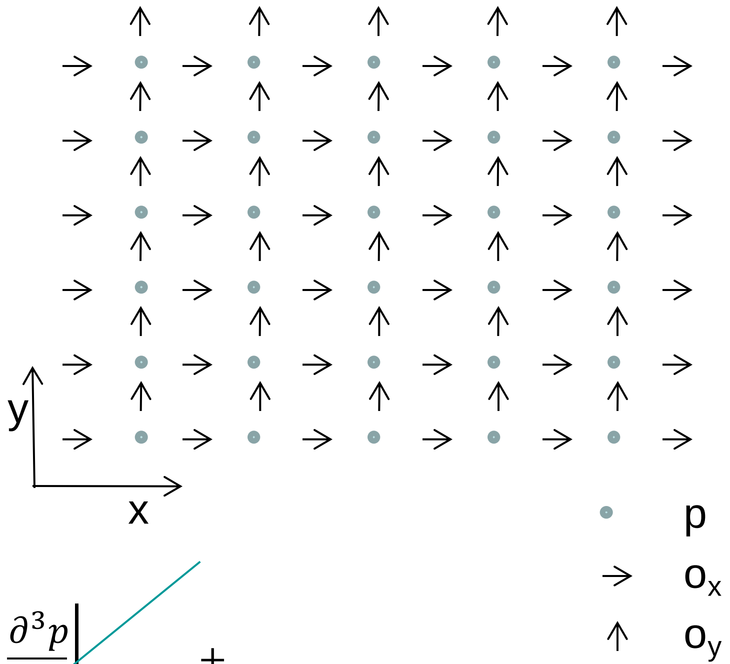
- Staggered grid
  - *p* and **o**-components discretised at locations shifted by half a grid step

$$p(idx, jdy, kdz)$$
$$o_x((i + {}^{1}/_{2})dx, jdy, kdz), \ldots$$

  - For updating o_x, time derivative at (*i*+1/2, *j*, *k*)
  - Via equation -> spatial derivative

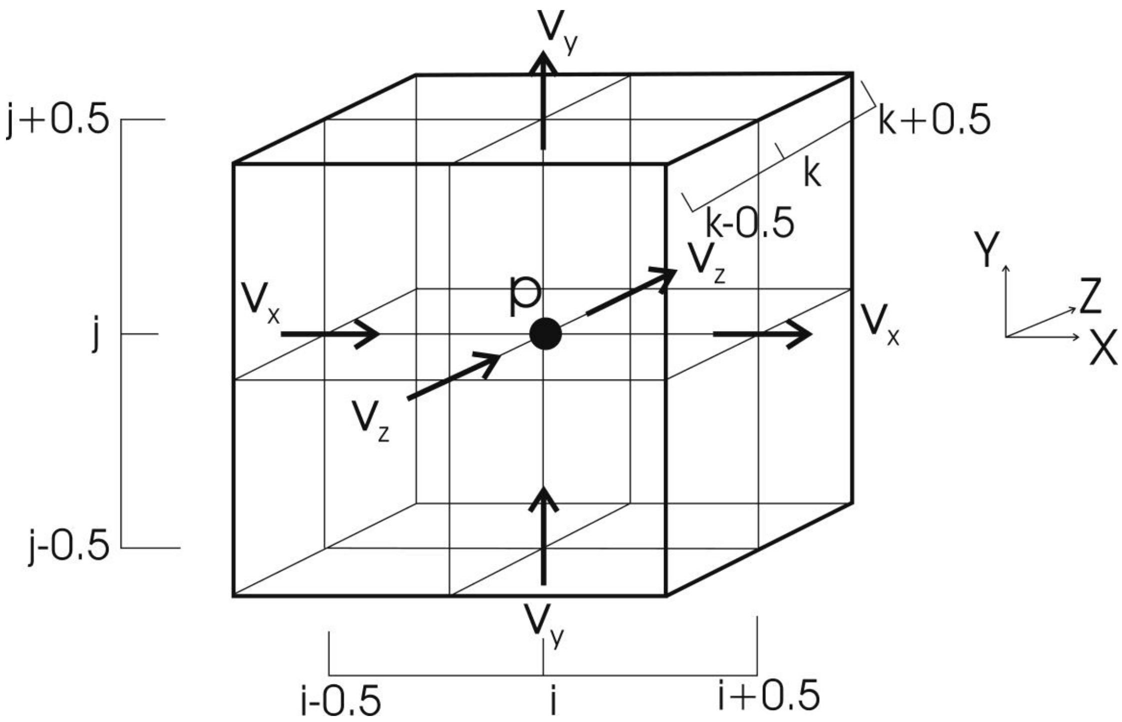
$$\left.\frac{\partial p}{\partial x}\right|_{x_0 + {}^{dx}/_{2}} = \frac{1}{dx}\left(p(x_0 + dx) - p(x_0)\right) + \cancel{\frac{dx^2}{4.3!}\left.\frac{\partial^3 p}{\partial x^3}\right|_{x_0 + {}^{dx}/_{2}}} + \ldots$$

  - Smaller error!
  - Nearest neighbors used -> no gaps -> small size problem eliminated
  - Miss-fit for some additional terms (see later)



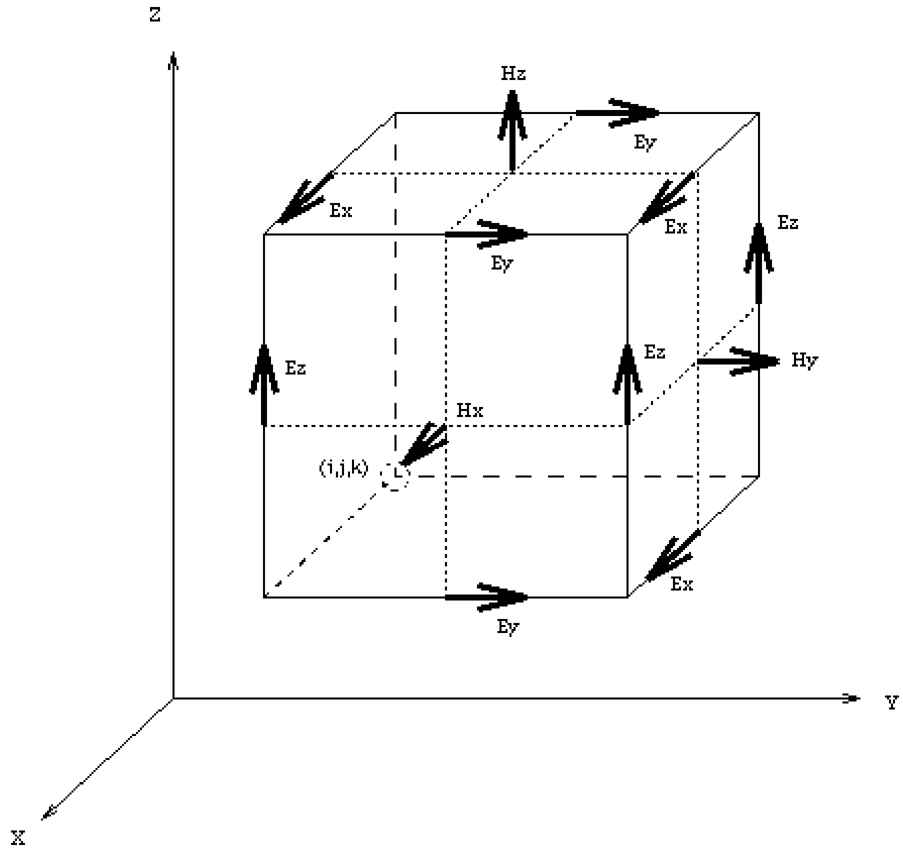
1.a) Cartesian grids

- Staggered grids in 3D
  - General equation & acoustic



1.a) Cartesian grids

- Electromagnetic using **E** and **H**
  - Yee-cell



  - Look at $\mu\frac{\partial H_x}{\partial t} = -\nabla\times\mathbf{E}\Big|_x = \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y}$ to see that discretisation fits!

1.b) Extended stencils

- Idea: improve accuracy of numerical approximation to spatial derivative
  - By including more terms in the series expansion and including points that are further away, one can easily derive higher order approximations for the spatial derivatives
  - E.g. 7 points in collocated grid

$$\left.\frac{\partial p}{\partial x}\right|_{x_0} = \frac{p(x_0+3dx) - 9p(x_0+2dx) + 45p(x_0+dx) - 45p(x_0-dx) + 9p(x_0-2dx) - p(x_0-3dx)}{60dx} + O(dx^6)$$

$$\left.\frac{\partial p}{\partial x}\right|_{x_0} \cong \frac{1}{dx}\sum_{i=-n}^{n} a_i p(x_0 + idx)$$

  - The phase error of this scheme can further be improved by minimizing phase error by tuning a_i. This leads to Dispersion Relation Preserving (DRP) schemes.
- Problem: boundaries, sources, ... so only useful for simple geometry.

1.b) Extended stencils

- Finite element time domain (FETD) methods also aim at reducing the spatial sampling rate.
  - For a discussion on FE see next chapter.

1.b) Extended stencils

- Pseudo Spectral Time Domain
  - Projection of *p*(*x*,*t*) on set of orthogonal basis functions

$$p(x,t) = \sum_{|n|<\infty} P_n(t)\Psi_n(x)$$

- Fourier Pseudo Spectral Time Domain
  - Basis functions are sine functions and Fourier transform can be used

$$p(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} P(k,t)\, e^{jkx}\, dk \qquad \text{with} \qquad P(k,t) = \int_{-\infty}^{\infty} p(x,t)\, e^{-jkx}\, dx$$

  - Spatial derivative can be calculated as

$$\frac{\partial p(x,t)}{\partial x} = \frac{1}{2\pi}\int_{-\infty}^{\infty} jkP(k,t)\, e^{jkx}\, dk$$

  - After discretisation

$$p_i(t) \overset{FFT}{\rightarrow} P_k(t) \overset{\times jk}{\rightarrow} jkP_k(t) \overset{IFFT}{\rightarrow} \left.\frac{\partial p(t)}{\partial x}\right|_i$$

1.b) Extended stencils

- Fourier Pseudo Spectral Time Domain
  - Accurate until Nyquist sampling limit (2 point per λ)
  - Extended scheme complicates implementation boundary conditions
  - Gibbs phenomenon at sharp discontinuities between materials
- Extended Fourier PS method
  - Alternative basis functions to avoid Gibbs phenomenon
  - Assuming interface between materials at x=0

$$\psi_+(\epsilon,x) = N_+(\epsilon)\begin{cases} \alpha_1 e^{\frac{\sqrt{\epsilon}}{c_1}x} + \beta_1 e^{-\frac{\sqrt{\epsilon}}{c_1}x} & x \le 0 \\ e^{\frac{\sqrt{\epsilon}}{c_2}x} & x \ge 0, \end{cases}$$

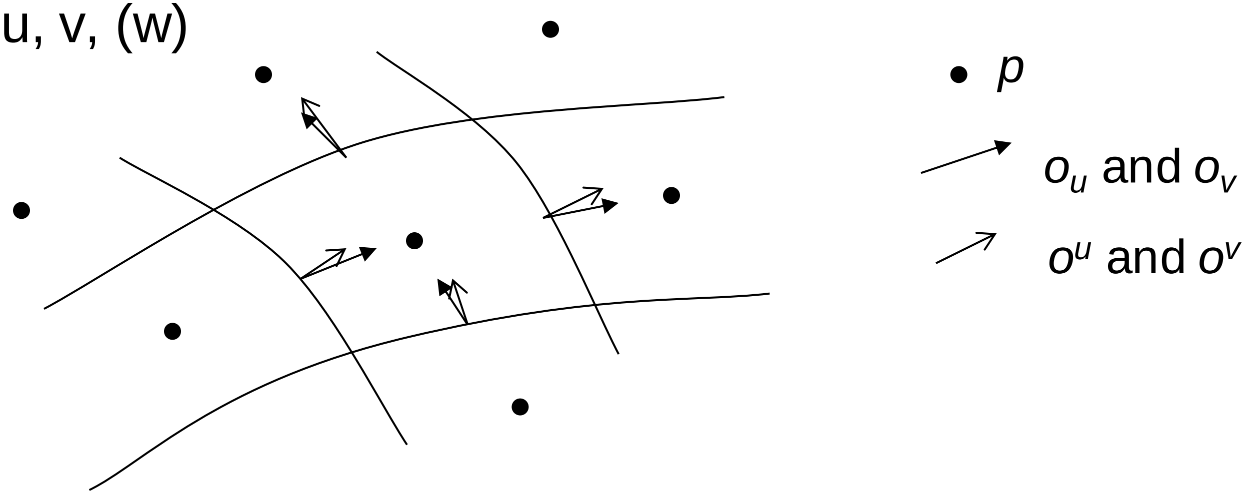
$$\psi_-(\epsilon,x) = N_-(\epsilon)\begin{cases} e^{-\frac{\sqrt{\epsilon}}{c_1}x} & x \le 0 \\ \alpha_2 e^{-\frac{\sqrt{\epsilon}}{c_2}x} + \beta_2 e^{\frac{\sqrt{\epsilon}}{c_2}x} & x \ge 0, \end{cases}$$

plane waves!

  - α and β follow from continuity condition at x=0; *N* from orthogonality
  - $\epsilon = -k_j^2 c_j^2,$
  - FFT can still be used, thus fast, but method is less general

1.c) Non-Cartesian structured grids

- Structured grids
  - Can be mapped one-to-one on Cartesian
- Curvilinear grids
  - Coordinates u, v, (w)



  - Vector can be expanded in covariant $\mathbf{e}_u$, … and in contravariant unit vectors $\mathbf{e}^u$, …

$$\mathbf{o} = o_u \mathbf{e}^u + o_v \mathbf{e}^v + o_w \mathbf{e}^w = o^u \mathbf{e}_u + o^v \mathbf{e}_v + o^w \mathbf{e}_w$$

  - Component are related via the metric coefficients + interpolation

$$o_u = \sum_i g_{ui} o^i; \quad o^u = \sum_i g^{ui} o_i$$

1.c) Non-Cartesian structured grids

- Curvilinear grids (continued)
  - Covariant components are naturally derived from

$$\frac{\partial o_u}{\partial t} = -\frac{\partial p}{\partial u}$$

  - Contravariant components (orthogonal to grid planes) are needed to calculate

$$\frac{\partial p}{\partial t} = -c^2\left(\frac{\partial o^u}{\partial u} + \frac{\partial o^v}{\partial v} + \frac{\partial o^w}{\partial w}\right)$$

  - Simplest approach:
    - Calculate covariant components of **o** using a first order finite difference discretisation of spatial derivatives
    - Transform to contravariant
    - Calculate *p*
  - Several variants were developed

1.c) Non-Cartesian structured grids

- Curvilinear grid for **E** and **H** fields
  - Looking at the Maxwell's equations
    - if components of **E** and **H** are chosen along covariant
    - **D** and **B** components along contravariant is natural choice

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + j$$

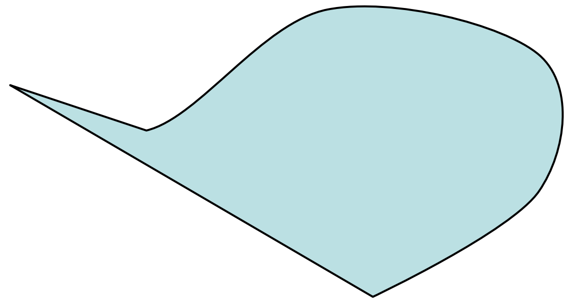
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \cdot \mathbf{D} = \rho$$

$$\nabla \cdot \mathbf{B} = 0$$

1.d) Non-structured grids

- Problem: objects with complicated form

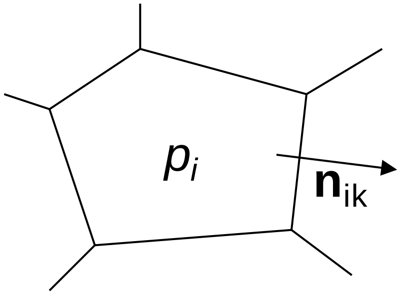


- Proposed approach: finite volume
  - Resolve one of the two equations by definition of unknowns
  - Conservation form by integrating $\frac{\partial p}{\partial t} + c^2 \nabla \cdot \mathbf{o} = 0$ over one cell

$$\int_{V_i} \frac{\partial p}{\partial t} dV = c^2 \int_{V_i} \nabla \cdot \mathbf{o} dV = c^2 \sum_k \int_{S_{ik}} \mathbf{o} \cdot \mathbf{n}_{ik} dS$$

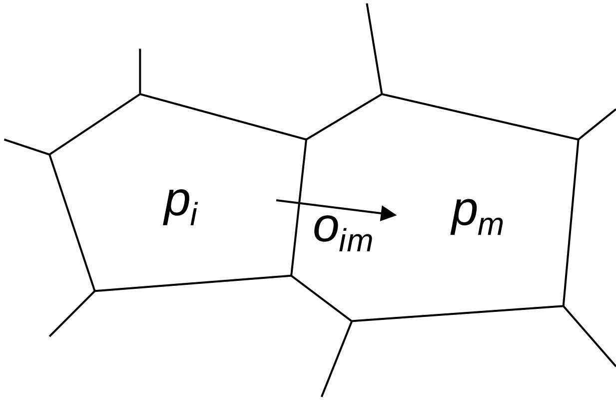
  - With new unknowns

$$p_i := \frac{1}{V_i} \int_{V_i} p dV; \quad o_{ik} := \frac{1}{S_{ik}} \int_{S_{ik}} \mathbf{o} \cdot \mathbf{n}_{ik} dS; \quad \frac{\partial p_i}{\partial t} \boxed{= -c2 \sum_k \frac{S_{ik}}{V_i} o_{ik}}$$



1.d) Non-structured grids

- Proposed approach (continued)
  - Integrate orthogonal component of $\frac{\partial \mathbf{o}}{\partial t} + \nabla p = 0$ over surface S_{im}

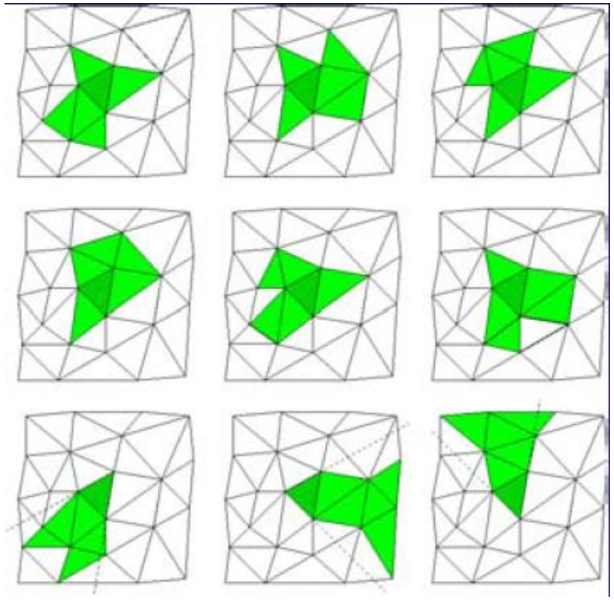


$$\frac{\partial o_{im}}{\partial t} = \frac{1}{S_{im}} \int_{S_{im}} \frac{\partial \mathbf{o}}{\partial t} \cdot \mathbf{n}_{im} dS = -\frac{1}{S_{im}} \int_{S_{im}} \frac{\partial p}{\partial n_{im}} dS$$

  - Which reduces the problem to approximating the *p* field locally by an analytical function and calculating the normal derivative.
  - The lowest order approximation = linear gradient in the direction $\mathbf{n}_{im}$
  - This results in $\boxed{\frac{\partial o_{im}}{\partial t} = -\frac{1}{d_m + d_i}(p_m - p_i)}$
  - With d_i and d_m the distance between the center of gravity of cell *i* and *m* and the plane of S_{im}

1.d) Non-structured grids

- Proposed approach (continued)
  - Higher order approximations expand *p* in polynomial around S_{im}
  - Match with suitable neighboring cells = stencil
  - E.g.



  - This leads to ENO (Essentially Non-Oscillating) and WENO (Weighted ...) schemes. Very popular when shock needs to be captured

2. Explicit, implicit, and stability

a) Explicit, leap-frog, staggered in time
b) Stability, Courant limit
c) Explicit Runge Kutta
d) Implicit time stepping, Crank Nicolson
e) Closure

2.a) Explicit, leap-frog, staggered in time

- The time dimension is investigated for Cartesian grid and staggered in space discretisation
- Time discretisation
  - Collocated in time: *p* and **o** are discretised at *t*=*l dt*
  - Staggered in time: *p* is discretised at *t*=*l dt* and **o** at *t*=(*l*+1/2) *dt*
  - As for spatial derivatives, approximating time derivatives by central differences based on a staggered grid is advantageous

$$\frac{1}{dt}\left(p((l+1)dt) - p(ldt)\right) = -c^2\, \nabla\cdot\mathbf{o}\Big|_{(l+1/2)dt}$$

$$\frac{1}{dt}\left(o_x((l+1/2)dt) - o_x((l-1/2)dt)\right) = -\frac{\partial p}{\partial x}\bigg|_{ldt}$$

- Solution mechanism: explicit, leap-frog

$$p((l+1)dt) = p(ldt) - c^2 dt\, \nabla\cdot\mathbf{o}\Big|_{(l+1/2)dt}$$

$$o_x((l+1/2)dt) = o_x((l-1/2)dt) - dt\frac{\partial p}{\partial x}\bigg|_{ldt}$$

2.a) Explicit, leap-frog, staggered in time

- Solution mechanism: explicit, leap-frog (continued)
  - The algorithm results in in-place computation = new values can replace old ones in computer memory. Huge advantage!
  - In natural way, left hand side is known (occurs earlier in time) before new values are calculated.
  - Additional terms in the equation may cause problem.
  - Stability not automatically guaranteed!

2.b) Stability, Courant limit

- The equations derived above are a special case of a Linear Time Invariant (LTI) system in discrete time
  - Assume only one time step delay $\mathbf{Y}(i) = \mathbf{A}\mathbf{Y}(i-1) + \mathbf{X}(i)$
  - Or after Z-transform

$$(\mathbf{1} - \mathbf{A}z^{-1})\mathbf{Y}(z) = \mathbf{X}(z)$$
$$\mathbf{Y}(z) = (\mathbf{1} - \mathbf{A}z^{-1})^{-1}\mathbf{X}(z)$$

  - This system is stable if the poles fall inside the unit circle or equivalently if all eigenvalues, λ_i, of **A** fulfill $|\lambda_i| \leq 1$
- For explicit (FDTD) scheme the matrix **A** can be constructed, and stability analyzed
  - **Y** is the vector of *p* and components of **o** at each discretisation point.
  - It is possible to include boundaries and additional terms

2.b) Stability, Courant limit

- Basic stability requirement for infinitely extended simulation area
  - Solve matrix with periodic extension
  - Analytical expression for stability condition can be derived easier based on spatial Fourier transform.

$$p(\mathbf{r},t) = \int \hat{p}(t) e^{-j\mathbf{k}\cdot\mathbf{r}} \mathbf{dk} \qquad \mathbf{o}(\mathbf{r},t) = \int \hat{\mathbf{o}}(t) e^{-j\mathbf{k}\cdot\mathbf{r}} \mathbf{dk}$$

  - Stability can be guaranteed by guaranteeing it for the integrand (every **k**)
  - Substitute in FDTD equations (Cartesian, staggered)

$$\hat{p}(t+dt)e^{-j\mathbf{k}\cdot\mathbf{r}_0} = \hat{p}(t)e^{-j\mathbf{k}\cdot\mathbf{r}_0} + \frac{c^2 dt}{dx}\left(\hat{o}_x(t+dt/2)e^{-j(\mathbf{k}\cdot\mathbf{r}_0 + k_x dx/2)} - \hat{o}_x(t+dt/2)e^{-j(\mathbf{k}\cdot\mathbf{r}_0 - k_x dx/2)}\right) + \ldots$$

  - After reduction

$$\hat{p}(t+dt) = \hat{p}(t) + \frac{c^2 dt}{dx}\hat{o}_x(t+dt/2)\left(e^{-jk_x dx/2} - e^{jk_x dx/2}\right) + \ldots$$

2.b) Stability, Courant limit

- Basic stability requirement (continued)
  - Similarly for o_x, o_y, ...

$$\hat{o}_x(t + dt/2) = \hat{o}_x(t - dt/2) + \frac{dt}{dx}\hat{p}(t)\left(e^{-jk_x dx/2} - e^{jk_x dx/2}\right)$$

  - We define the vector of discrete variables as

$$\mathbf{Y}(i) = \begin{bmatrix} p((i+1)dt) \\ o_x((i + {}^{1}/_{2})dt) \\ o_y((i + {}^{1}/_{2})dt) \\ o_z((i + {}^{1}/_{2})dt) \end{bmatrix}$$

  - Resulting in the system matrix

$$\mathbf{A} = \begin{bmatrix} 1 - \frac{c^2 dt^2}{dx^2} 4\sin^2\left(\frac{k_x dx}{2}\right) - \ldots & -\frac{c^2 dt}{dx} 2j\sin\left(\frac{k_x dx}{2}\right) & -\frac{c^2 dt}{dy} 2j\sin\left(\frac{k_y dy}{2}\right) & -\frac{c^2 dt}{dz} 2j\sin\left(\frac{k_z dz}{2}\right) \\ -\frac{dt}{dx} 2j\sin\left(\frac{k_x dx}{2}\right) & 1 & 0 & 0 \\ -\frac{dt}{dy} 2j\sin\left(\frac{k_y dy}{2}\right) & 0 & 1 & 0 \\ -\frac{dt}{dz} 2j\sin\left(\frac{k_z dz}{2}\right) & 0 & 0 & 1 \end{bmatrix}$$

2.b) Stability, Courant limit

- Basic stability requirement (continued)
  - One easily verifies that the eigenvalues of **A** are 1 or solution of

$$\lambda^2 - (2 - \alpha_x - \alpha_y - \alpha_z)\lambda + 1 = 0$$
$$\alpha_x = \frac{4c^2 dt^2}{dx^2} \sin^2\left(\frac{k_x dx}{2}\right)$$

  - These solutions are

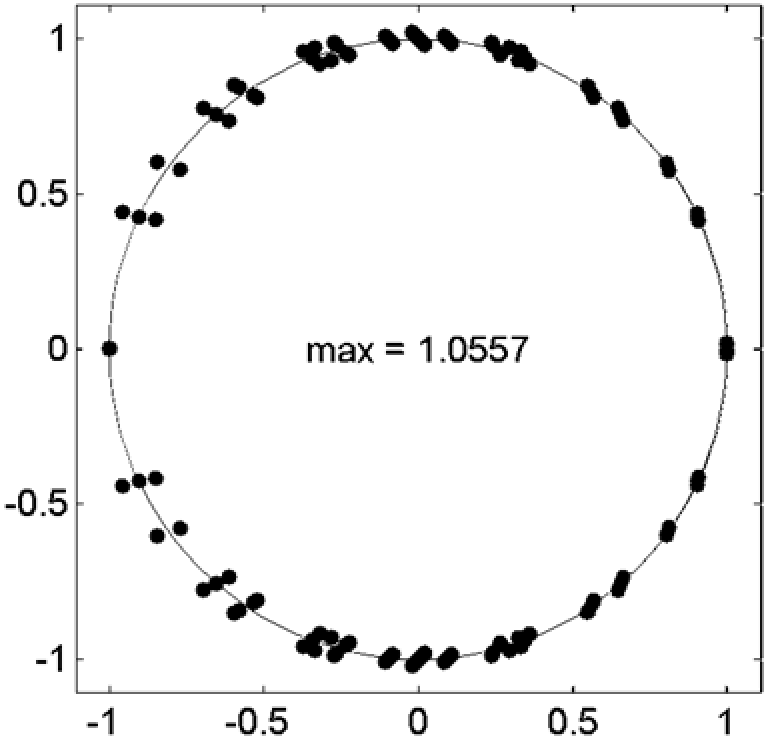
$$\lambda_{\pm} = \frac{(2 - \alpha_x - \alpha_y - \alpha_z) \pm \sqrt{(\alpha_x + \alpha_y + \alpha_z)(\alpha_x + \alpha_y + \alpha_z - 4)}}{2}$$

    - If $(\alpha_x + \alpha_y + \alpha_z) > 4$, the eigenvalues are real and one of them is smaller than -1 so the system is unstable
    - If $(\alpha_x + \alpha_y + \alpha_z) < 4$, the eigenvalues are complex conjugate with product equal to 1 so the system is stable
    - For the equality both eigenvalues are -1 also resulting in a stable system
  - Since $(\alpha_x + \alpha_y + \alpha_z) \leq 4$ should hold for all k, $\boxed{c^2 dt^2\left(\frac{1}{dx^2} + \frac{1}{dy^2} + \frac{1}{dz^2}\right) \leq 1}$
  - This is Courant stability condition

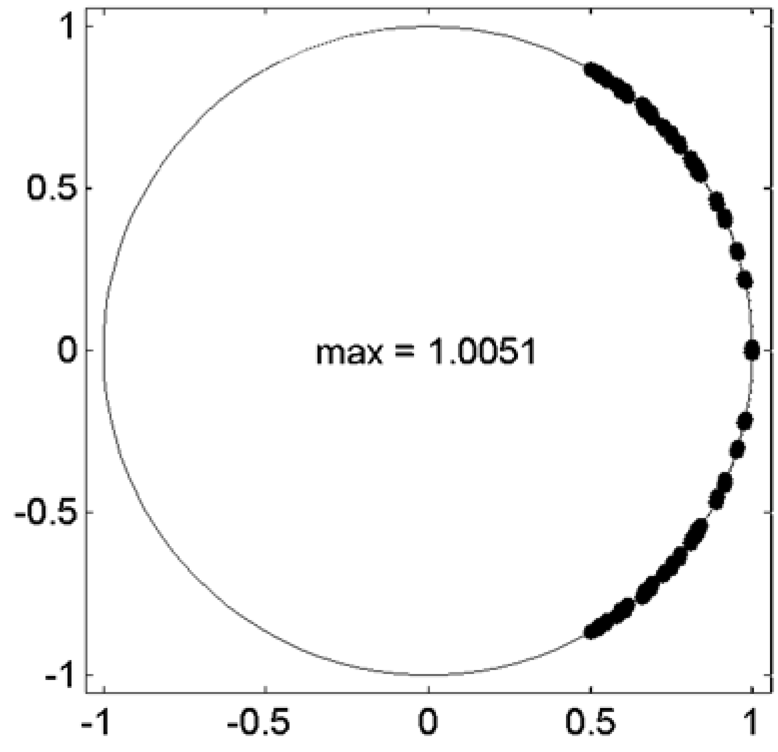
2.b) Stability, Courant limit

- Example of application of stability analyses

Slightly unstable due to moving system, M=0.05, CN=1



Improved stability by reducing CN, M=0.05, CN=0.5



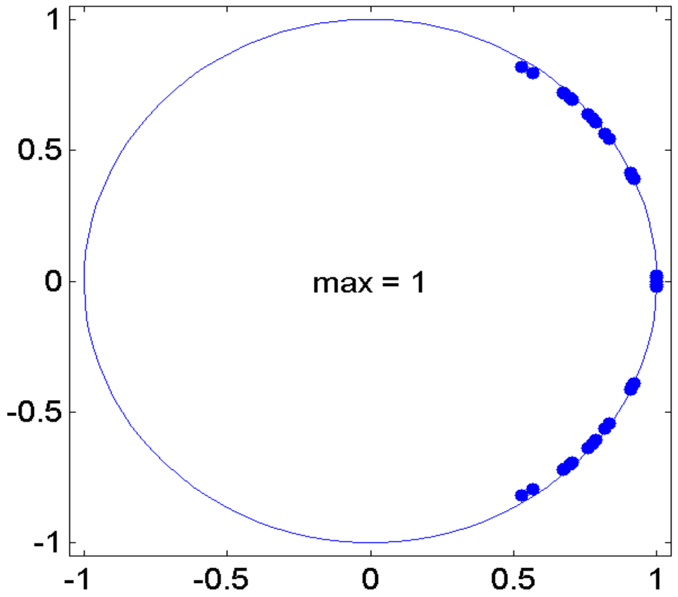
2.c) Explicit Runge Kutta

- Higher order approximation to time integration
  - Dual to higher order approximation to spatial derivative
  - After spatial discretisation, equations can be written as

$$\frac{\partial \mathbf{Y}(t)}{\partial t} = \mathbf{B} \cdot \mathbf{Y}(t) + \mathbf{X}(t)$$

  - Runge-Kutta introduces several intermediate steps in one step *dt*
  - RK of order three (for example)

$$\mathbf{Y}^{(1)}(t) = \mathbf{Y}(t) + dt\mathbf{B} \cdot \mathbf{Y}(t)$$
$$\mathbf{Y}^{(2)}(t) = \frac{3}{4}\mathbf{Y}(t) + \frac{1}{4}\mathbf{Y}^{(1)}(t) + \frac{1}{4}dt\mathbf{B} \cdot \mathbf{Y}^{(1)}(t)$$
$$\mathbf{Y}(t+dt) = \mathbf{Y}^{(3)}(t) = \frac{1}{3}\mathbf{Y}(t) + \frac{2}{3}\mathbf{Y}^{(2)}(t) + \frac{2}{3}dt\mathbf{B} \cdot \mathbf{Y}^{(2)}(t)$$



  - Time step is usually small enough
  - Stability slightly better in some cases

2.d) Implicit time stepping, Crank Nicolson

- Crank Nicolson time discretisation
  - After spatial discretisation of the wave equations, the continuous time system can be written as

$$\frac{\partial \mathbf{Y}(t)}{\partial t} = \mathbf{B} \cdot \mathbf{Y}(t) + \mathbf{X}(t)$$

  - In Laplace domain the system is described by

$$s\mathbf{Y}(s) = \mathbf{B} \cdot \mathbf{Y}(s) + \mathbf{X}(s)$$
$$(\mathbf{B} - s\mathbf{I})\mathbf{Y}(s) = -\mathbf{X}(s)$$

  - This system is stable (since it is a physical system) thus the poles of $(\mathbf{B} - s\mathbf{I})$ are located left of the imaginary axes or on it
  - Could one find a time sampling of this system that maps the left of the imaginary axes inside the unit circle and thus results in an unconditionally stable system?

2.d) Implicit time stepping, Crank Nicolson

- Crank Nicolson time discretisation (continued)
  - Suggested transform to Z-domain $s = \frac{2}{dt}\frac{1-z^{-1}}{1+z^{-1}}$

    $$z = \frac{1+{}^{dt}/_{2}\,s}{1-{}^{dt}/_{2}\,s}$$

  - Check that pole at s=-|r|+$j\omega$ corresponds to point inside unit circle in Z-domain after this transform!
  - Time discretisation (using this technique) of wave equation results in

$$(1-z^{-1})\mathbf{Y}(z) = \frac{dt}{2}(1+z^{-1})\mathbf{B}\cdot\mathbf{Y}(z) + \frac{dt}{2}(1+z^{-1})\mathbf{X}(z)$$

or $$\left(1-\frac{dt}{2}\mathbf{B}\right)\mathbf{Y}(z) = \left(1+\frac{dt}{2}\mathbf{B}\right)z^{-1}\mathbf{Y}(z) + \frac{dt}{2}(1+z^{-1})\mathbf{X}(z)$$

  - And in discrete time

$$\left(1-\frac{dt}{2}\mathbf{B}\right)\mathbf{Y}(i) = \left(1+\frac{dt}{2}\mathbf{B}\right)\mathbf{Y}(i-1) + \frac{dt}{2}\left(\mathbf{X}(i)+\mathbf{X}(i-1)\right)$$

2.d) Implicit time stepping, Crank Nicolson

- Implicit scheme

$$\left(1-\frac{dt}{2}\mathbf{B}\right)\mathbf{Y}(i)=\left(1+\frac{dt}{2}\mathbf{B}\right)\mathbf{Y}(i-1)+\frac{dt}{2}\left(\mathbf{X}(i)+\mathbf{X}(i-1)\right)$$

  – The matrix preceding **Y** is sparse and therefore the set of equations can be solved efficiently
  – Slightly more memory than explicit scheme
  – CPU-time comparison depends on various factors
    - Structure
    - Required accuracy

2.e) Closure

- Staggered Cartesian grid with first order finite-difference in space and time
  - Is in many aspects an optimal point
  - Is very popular because of the beauty that lies in its simplicity
- Other schemes should be investigated for specific purposes

3. Numerical accuracy

a) Accuracy of basic FDTD scheme
b) DRP schemes

3.a) accuracy of basic FDTD scheme

- Analytical expression for FDTD in staggered Cartesian grid
  - Amplitude and phase error for plane wave
  - Since poles of **A** are located on the unit circle, the system is all-pass, so amplitude is conserved.
  - This is easily verified by proposing $\begin{bmatrix} \hat{p}(t) \\ \hat{o}_x(t) \\ \hat{o}_y(t) \\ \hat{o}_z(t) \end{bmatrix} = \begin{bmatrix} \hat{P} \\ \hat{O}_x \\ \hat{O}_y \\ \hat{O}_z \end{bmatrix} e^{j\phi(t)} = \mathbf{Y}e^{j\phi(t)}$
  - Note that $\varphi(t)=\omega t$ if no phase error would occur
  - Substitution in the general system equation results in $\left(\mathbf{A} - e^{j\Delta\phi}\,\mathbf{I}\right)\mathbf{Y} = 0$
  - With $\Delta\varphi$ the change in phase during one time step
  - This homogeneous equation has a solution if $\det\left(\mathbf{A} - e^{j\Delta\phi}\,\mathbf{I}\right) = 0$
  - Precisely the eigenvalue equation, thus

$$e^{j\Delta\phi} = \frac{(2 - \alpha_x - \alpha_y - \alpha_z) \pm \sqrt{(\alpha_x + \alpha_y + \alpha_z)(\alpha_x + \alpha_y + \alpha_z - 4)}}{2}$$

3.a) accuracy of basic FDTD scheme

- Analytical expression (continued)
  - To extract phase, add complex conjugate

$$2\cos(\Delta\phi) = e^{j\Delta\phi} + e^{-j\Delta\phi} = 2 - (\alpha_x + \alpha_y + \alpha_z)$$

$$\sin^2(\frac{\Delta\phi}{2}) = \frac{(\alpha_x + \alpha_y + \alpha_z)}{4}$$

$$\Delta\phi = 2\arcsin\left(c\ dt\sqrt{\frac{\sin^2(k_x dx/2)}{dx^2} + \frac{\sin^2(k_y dy/2)}{dy^2} + \frac{\sin^2(k_z dz/2)}{dz^2}}\right)$$

  - Note that the phase is exactly ωdt for CN=1 and diagonal propagation
- In general: compare to amplitude and phase of known solution

3.b) DRP scheme

– Consider again the extended stencil for spatial discretisation

$$\left.\frac{\partial p}{\partial x}\right|_{x_0} \cong \frac{1}{dx}\sum_{i=-n}^{n} a_i p(x_0 + idx)$$

– Apply spatial Fourier transform to both sides

$$jk\hat{p} \cong \frac{1}{dx}\sum_{i=-n}^{n} a_i e^{jkidx}\hat{p}$$

– Call α the FDTD approximation to the wave number *k*

$$\alpha = \frac{-j}{dx}\sum_{i=-n}^{n} a_i e^{jkidx}$$

– We can now minimize the difference between *k* and α in a given interval

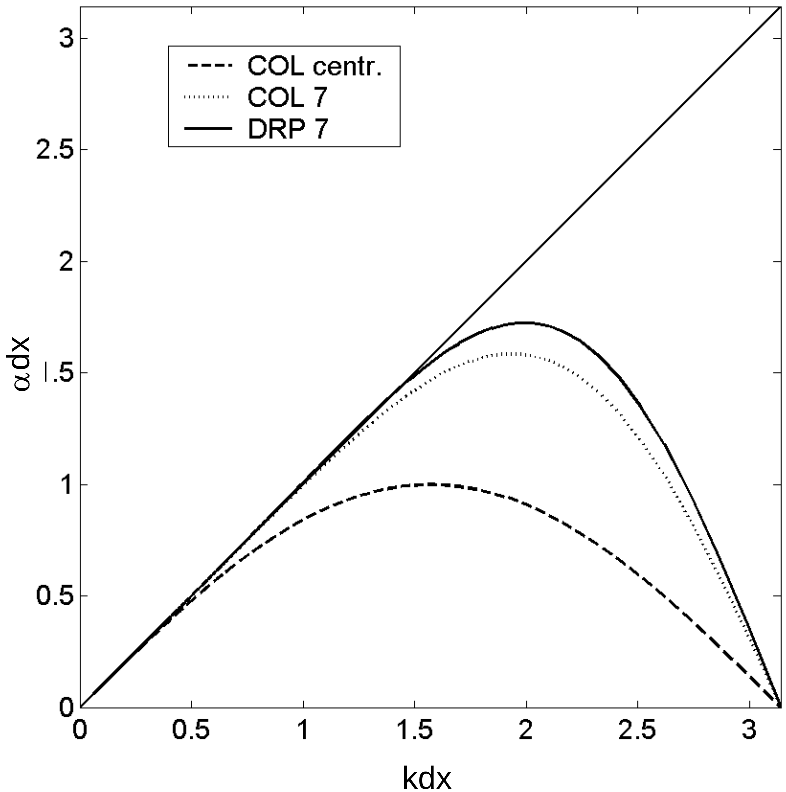
$$e = \int_{-\pi/2}^{\pi/2} |\alpha dx - kdx|^2 d(kdx)$$

– This gives a set of equations that can be solved for a_i (assume a_i=-a_{-i})

3.b) DRP scheme

– Example: n=3, 7-point stencil in collocated grid

$$a_0 = 0 \qquad a_1 = a_{-1} = 0.79926643$$
$$a_2 = a_{-2} = -0.18941314 \qquad a_3 = a_{-3} = 0.02651995$$

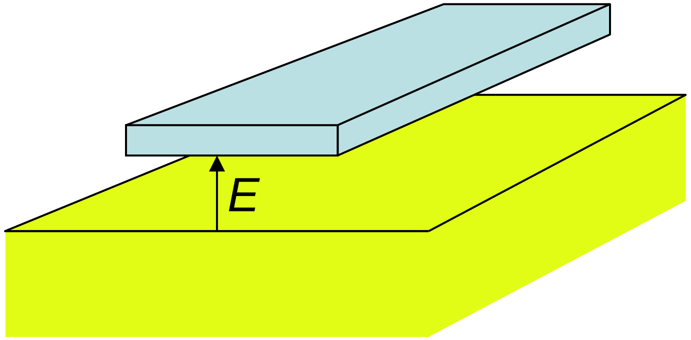


4. Sources and boundary conditions

a) Non-transparent sources
b) Transparent sources
c) Impedance boundary conditions

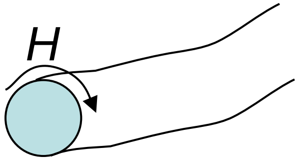
4.a) non-transparent sources

- Orthogonal component of **o** forced
  - Example: vibrating surface as acoustic source
  - Easy to implement $o_n=f(t)$ if surface is grid plane
  - Note that the boundary correspond to hard boundary $o_n=0$ for incoming wave
- Tangential component of electric field ($\mathbf{o}_t$ or p in 2D problem)
  - Example: electric field in slot or via-hole
    - PEC for incoming wave
  - Example: voltage at start of interconnect
    - Short circuit for incoming wave
- Tangential magnetic field
  - Example: current in conductor



$V = \int E dl$

$I = \oint H dl$



4.b) transparent sources

- Added to *p* update equation
  - Monopole point source
  - Note that source size is actually one grid cell volume
- Added to update equation for one of the components of **o**
  - Dipole point source
  - Note that source size is actually one grid cell surface
- Add current to *E* update equation
- Initial field
  - Example incoming plane wave of finite duration

4. sources

- Which time dependence should be used if interest is in frequency response
  - Problem: strong peaks outside area of interest may show side lobes due to finite length of time sequence that is Fourier transformed (FFT)
  - Limit stimulus energy outside region of interest
  - Example

$$f(t) = (t - t_0) \exp\left(\frac{-(t - t_0)^2}{\sigma^2}\right)$$

    - No DC
    - σ^2 allows to tune bandwidth
  - Example

$$f(t) = \sin(2\pi f_0 (t - t_0)) \exp\left(\frac{-(t - t_0)^2}{\sigma^2}\right)$$

    - “narrow” band centered around f_0

4.c) impedance boundary

- Real surface impedance $p = Z_R o_n$
  - Implemented at plane where o_n is discretised, assume o_x with impedance for larger x, boundary at $i_0+1/2$
  - Shift unknown p to surface

$$o_x^{\ell+1/2}(i_0 + {}^1/_2) = o_x^{\ell-1/2}(i_0 + {}^1/_2) - \frac{2dt}{dx}\left(p^\ell(i_0 + {}^1/_2) - p^\ell(i_0)\right)$$

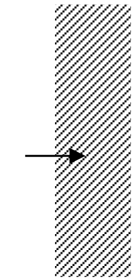
  - Resolve unknown p at half grid step using impedance condition

$$o_x^{\ell+1/2}(i_0 + {}^1/_2) = o_x^{\ell-1/2}(i_0 + {}^1/_2) - \frac{2dt}{dx}\left(Z_R o_x^{\ell}(i_0 + {}^1/_2) - p^\ell(i_0)\right)$$

  - Resolve time mismatch for o_x by linear interpolation in time

$$\left(1 + \frac{Z_R dt}{dx}\right) o_x^{\ell+1/2}(i_0 + {}^1/_2) = \left(1 - \frac{Z_R dt}{dx}\right) o_x^{\ell-1/2}(i_0 + {}^1/_2) + \frac{2dt}{dx} p^\ell(i_0)$$

  - This approach does not restrict stability condition (as long as $Z_R \geq 0$)
    - $Z_R=0$ is equivalent to $p=0$ and results in perfect reflection
    - $Z_R=\infty$ is equivalent to $o_x=0$ and results in perfect reflection
    - Z_R=characteristic impedance (=c) absorbs an orthogonal plane wave



4.c) impedance boundary

- Complex surface impedance $\hat{P} = Z(\omega)\hat{O}_n$
  - Explicit convolution $p = \int Z(t-\tau)\, o_n(\tau) d\tau; \quad Z(t) = \int Z(\omega) e^{j\omega t} d\omega$
    - In most cases slow and memory consuming
    - Exception: $Z(t) = \frac{1}{t_0} e^{-t/t_0}$
  - Series expansion $\hat{P} = \frac{1}{j\omega} Z_{-1}\hat{O}_n + Z_0\hat{O}_n + j\omega Z_1 \hat{O}_n$
    - In time domain $p = Z_{-1}\int o_n dt + Z_0 o_n + Z_1 \frac{\partial o_n}{\partial t}$
    - In a similar way as for a real impedance one obtains

$$\left(1 + \frac{Z_0 dt}{dx} + \frac{2Z_1}{dx}\right) {o_x}^{\ell+1/2}(i_0 + \frac{1}{2}) = \left(1 - \frac{Z_0 dt}{dx} + \frac{2Z_1}{dx}\right) {o_x}^{\ell-1/2}(i_0 + \frac{1}{2}) + \frac{2dt}{dx} p^{\ell}(i_0) - \frac{2Z_{-1}dt}{dx} I^{\ell}(i_0 + \frac{1}{2})$$

$$I^{\ell}(i_0 + {}^{1}/_{2}) = I^{\ell-1}(i_0 + {}^{1}/_{2}) + {o_x}^{\ell-1/2}(i_0 + {}^{1}/_{2}) dt$$

4.c) impedance boundary

- Complex surface impedance (continued)
  - Digital filter design
    - In Z-domain, fit

$$p(z) = \frac{\sum_i a_i z^{-i}}{\sum_i b_i z^{-i}} o_n(z)$$

    - Which corresponds in time domain to

$$\sum_i b_i p^{\ell-i} = \sum_i a_i {o_n}^{\ell-i}; \quad b_0 p^{\ell} = \sum_i a_i {o_n}^{\ell-i} - \sum_{i=1} b_i p^{\ell-i}$$

    - Several techniques are available to fit the constants *a* & *b* to a known spectral dependence
    - One option is to use bilinear transformation on frequency domain function

$$j\omega \rightarrow \frac{2}{dt}\frac{1 - z^{-1}}{1 + z^{-1}}$$

5. Perfectly absorbing layers

a) A simple first order approach
b) Perfectly matched layers (PML)

5.a) A simple first order approach

- Consider a plane wave hitting the surface at orthogonal direction
- If Z_R=Z_c, the characteristic impedance of the medium, then reflection coefficient is zero

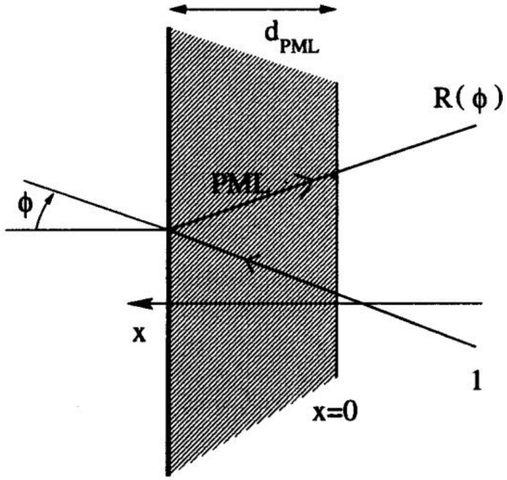
$$R = \frac{1 - \frac{Z}{Z_C}}{1 + \frac{Z}{Z_C}}$$

- But this does not work when angle of incidence is different

5.b) Perfectly matched layers (PML)

- Underlying idea
  - Include a layer with (increasing) damping but make sure no waves are reflected at its interface
  - Normally damping introduces *Z*, *k* different from free space and reflections occur
  - Additional freedom by splitting *p*

$$p = p_{\perp} + p_{//}$$



- Assuming α orthogonal to PML

$$\frac{\partial p_{\perp}}{\partial t} + c^2 \frac{\partial o_{\alpha}}{\partial \alpha} + \kappa_{1\perp} p_{\perp} = 0 \qquad (1)$$

$$\frac{\partial p_{//}}{\partial t} + c^2 \sum_{\gamma \neq \alpha} \frac{\partial o_{\gamma}}{\partial \gamma} + \kappa_{1//} p_{//} = 0 \qquad (2)$$

$$\frac{\partial o_{\alpha}}{\partial t} + \frac{\partial p}{\partial \alpha} + \kappa_{2\perp} o_{\alpha} = 0 \qquad (3)$$

$$\frac{\partial o_{\beta}}{\partial t} + \frac{\partial p}{\partial \beta} + \kappa_{2//} o_{\beta} = 0 \qquad \beta \neq \alpha \qquad (4)$$

5.b) Perfectly matched layers (PML)

- Perfect matching
  - All plane waves propagate undisturbed through the interface
  - Outside PML

$$p = p_0 e^{-jk\alpha\cos\theta - jk\beta\sin\theta} e^{-j\omega t}$$
$$o_\alpha = o_{0,\alpha} e^{-jk\alpha\cos\theta - jk\beta\sin\theta} e^{-j\omega t}$$
$$o_{0,\alpha} = -\frac{k\cos\theta}{\omega} p_0$$

  - Inside PML

$$p_\perp = p_{1,\perp} e^{-jk\alpha\cos\theta - jk\beta\sin\theta - \gamma_\alpha\alpha - \gamma_\beta\beta} e^{-j\omega t}$$
$$p_{//} = p_{1,//} e^{-jk\alpha\cos\theta - jk\beta\sin\theta - \gamma_\alpha\alpha - \gamma_\beta\beta} e^{-j\omega t}$$
$$o_\alpha = o_{1,\alpha} e^{-jk\alpha\cos\theta - jk\beta\sin\theta - \gamma_\alpha\alpha - \gamma_\beta\beta} e^{-j\omega t}$$

$$\xrightarrow{(3)} \quad o_{1,\alpha} = \frac{jk\cos\theta + \gamma_\alpha}{-j\omega + \kappa_{2,\perp}} (p_{1,\perp} + p_{1,//})$$

$$\xrightarrow{(4)} \quad o_{1,\beta} = \frac{jk\sin\theta + \gamma_\beta}{-j\omega + \kappa_{2,//}} (p_{1,\perp} + p_{1,//})$$

$$\xrightarrow{(1)} \quad (-j\omega + \kappa_{1,\perp}) p_{1,\perp} - c^2 \frac{(jk\cos\theta + \gamma_\alpha)^2}{-j\omega + \kappa_{2,\perp}} (p_{1,\perp} + p_{1,//}) = 0$$

$$\xrightarrow{(2)} \quad (-j\omega + \kappa_{1,//}) p_{1,//} - c^2 \frac{\left(jk\sin\theta + \gamma_\beta\right)^2}{-j\omega + \kappa_{2,//}} (p_{1,\perp} + p_{1,//}) = 0$$

5.b) Perfectly matched layers (PML)

- Perfect matching (continued)
  - This system of equations has a solution different from 0 only if the following determinant is zero

$$\begin{vmatrix} (-j\omega+\kappa_{1,\perp})-c^2\dfrac{(jk\cos\theta+\gamma_\alpha)^2}{-j\omega+\kappa_{2,\perp}} & -c^2\dfrac{(jk\cos\theta+\gamma_\alpha)^2}{-j\omega+\kappa_{2,\perp}} \\ -c^2\dfrac{\left(jk\sin\theta+\gamma_\beta\right)^2}{-j\omega+\kappa_{2,//}} & (-j\omega+\kappa_{1,//})-c^2\dfrac{\left(jk\sin\theta+\gamma_\beta\right)^2}{-j\omega+\kappa_{2,//}} \end{vmatrix}=0$$

  - Continuity at the interface of normal component of **o** and *p*

$$-\frac{k\cos\theta}{\omega}=\frac{jk\cos\theta+\gamma_\alpha}{-j\omega+\kappa_{2,\perp}} \qquad \gamma_\beta=0$$

  - thus

$$\begin{vmatrix} (-j\omega+\kappa_{1,\perp})-c^2(-j\omega+\kappa_{2,\perp})\left(-\dfrac{k}{\omega}\cos\theta\right)^2 & -c^2(-j\omega+\kappa_{2,\perp})\left(-\dfrac{k}{\omega}\cos\theta\right)^2 \\ -c^2(jk\sin\theta)^2 & (-j\omega+\kappa_{1,//})(-j\omega+\kappa_{2,//})-c^2(jk\sin\theta)^2 \end{vmatrix}=0$$

5.b) Perfectly matched layers (PML)

- Perfect matching (continued)
  - This must hold for all angles of the incident wave
  - It can be verified by matching terms or by just putting a few test values for θ (θ=0, θ=π/2)

$$(\kappa_{1,\perp} - \kappa_{2,\perp})(\kappa_{2,//} - j\omega)(\kappa_{1,//} - j\omega) = 0$$

$$\text{or } \kappa_{1,\perp} = \kappa_{2,\perp}$$

$$(\kappa_{1,\perp} - j\omega)\left[(\kappa_{1,//} - j\omega)(\kappa_{2,//} - j\omega) + \omega^2\right]$$
$$= 0$$
$$\text{or } \kappa_{1,//}\kappa_{2,//} - j\omega(\kappa_{1,//} + \kappa_{2,//}) = 0$$
$$\text{or } \kappa_{1,//} = 0 \text{ and } \kappa_{2,//} = 0$$

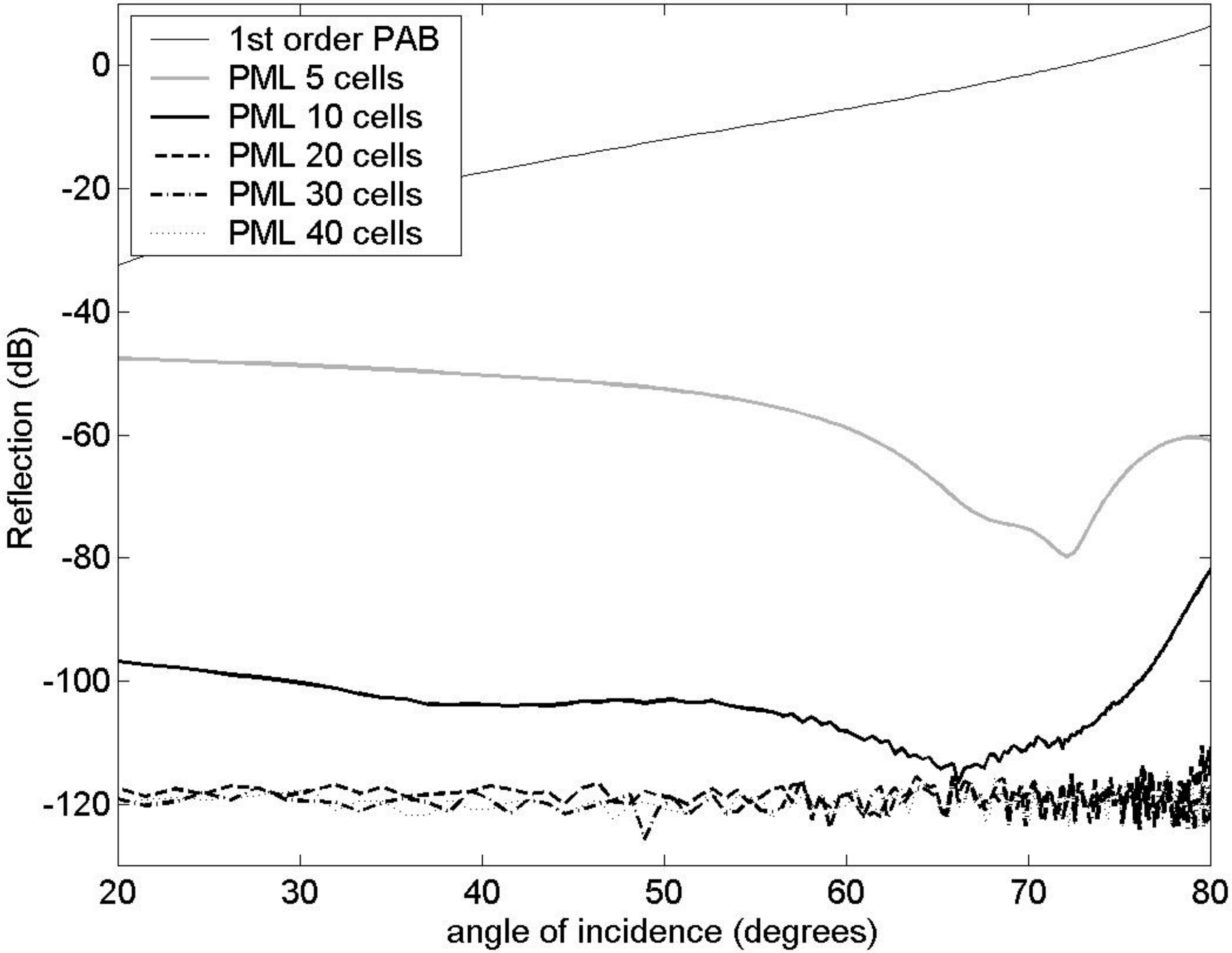
- Damping inside PML

$$\kappa_1(x) = \kappa_{1,MAX}\left(\frac{x}{d_{PML}}\right)^m$$

  - *m*=3 to 4 seems to work well
  - 10 to 40 layers

5.b) Perfectly matched layers (PML)

- Numerical example



6. Handling additional terms in the equation

a) Damping proportional to field
b) Damping proportional to derivative
c) Moving media

6.a) Damping proportional to field

– Discretise keeping in mind the staggering

$$\frac{\partial \mathbf{o}}{\partial t} + \nabla p + \kappa \mathbf{o} = 0$$

$$\frac{{o_x}^{\ell+1/2}(i+{}^1\!/_2) - {o_x}^{\ell-1/2}(i+{}^1\!/_2)}{dt} + \frac{p^{\ell}(i+1) - p^{\ell}(i)}{dx} + \kappa\frac{{o_x}^{\ell+1/2}(i+{}^1\!/_2) + {o_x}^{\ell-1/2}(i+{}^1\!/_2)}{2} = 0$$

$${o_x}^{\ell+1/2}(i+{}^1\!/_2) = \left(\frac{1-\kappa dt/2}{1+\kappa dt/2}\right){o_x}^{\ell-1/2}(i+{}^1\!/_2) - \frac{dt}{dx(1+\kappa dt/2)}\left(p^{\ell}(i+1) - p^{\ell}(i)\right)$$

6.b) Damping proportional to derivative

- Discretisation of second order derivative involves neighboring field values

$$\frac{\partial \mathbf{o}}{\partial t} + \nabla p + \mu \nabla^2 \mathbf{o} = 0$$

- Explicit scheme is not possible in staggered grid unless time discretisation is violated

6.c) Moving media

- Uniform movement or first approximation to general flow

$$\frac{\partial \mathbf{o}}{\partial t} - (\mathbf{v}_0 \cdot \nabla)\mathbf{o} + \nabla p = 0$$

and simular for *p*

  - Staggered grid does not result in explicit scheme unless discretisation strategy is violated, but this results in (slightly) unstable system
  - Collocation in time solves the problem, but more memory needed

$$o_x{}^{\ell+1}(i+{}^1/_2) = o_x{}^{\ell-1}(i+{}^1/_2) - v_{0x}\frac{dt}{2dx}\left(o_x{}^{\ell}(i+{}^3/_2) - o_x{}^{\ell}(i-{}^1/_2)\right) - v_{0y}\frac{dt}{2dy}\left(o_x{}^{\ell}(i+{}^1/_2, j+1) - o_x{}^{\ell}(i+{}^1/_2, j-1)\right) - \frac{dt}{dx}\left(p^{\ell}(i+1) - p^{\ell}(i)\right)$$

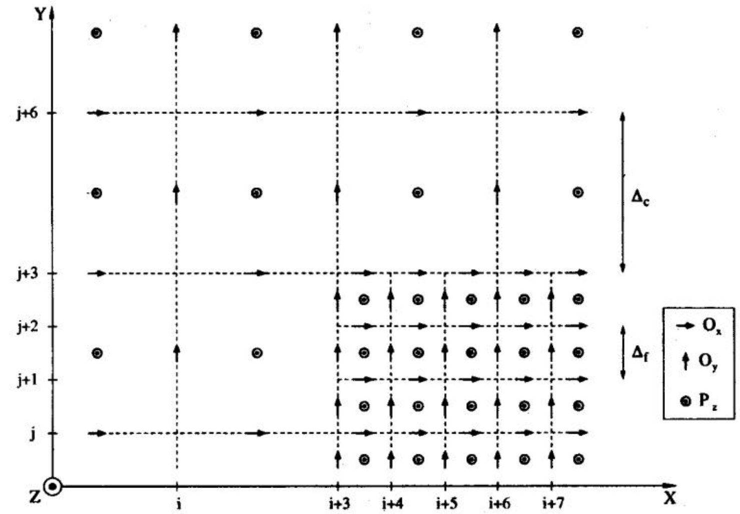
and simular for *p*

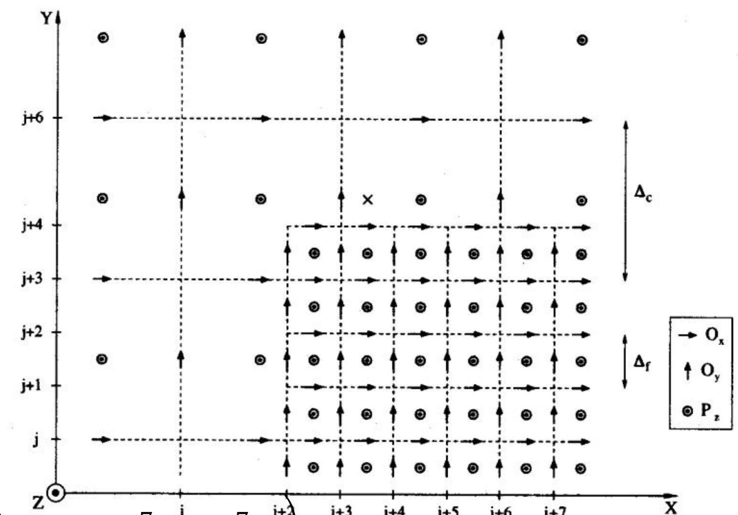
7. Grid refinement and subgridscale models

a) Problem statement
b) Cartesian refinement
c) Non-Cartesian matching
d) Small objects and openings
e) Boundary layers

7.b) Cartesian refinement

- Odd refinement ratios provide value in center of coarse cell so standard central difference is still possible in coarse grid cell close to interface
- Shifted fine grid also results in central difference approach for at least central cell
- Linear interpolation can be used as a first approach to calculate missing values, e.g.

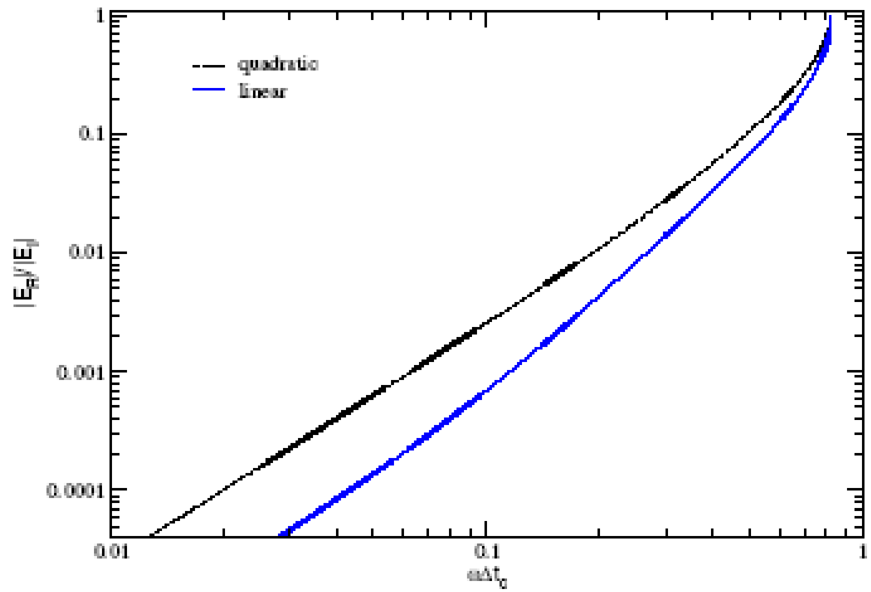




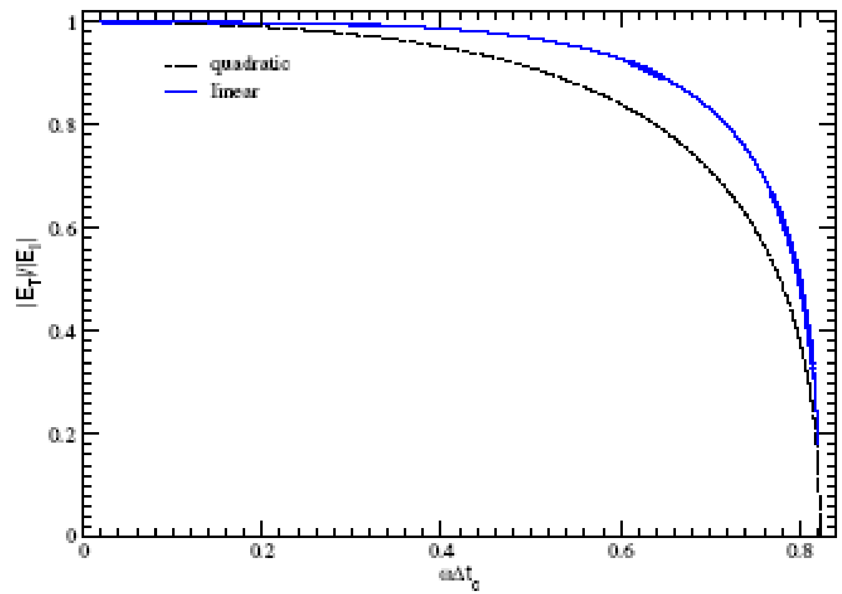
$$\left.\frac{\partial p}{\partial y}\right|_{i+7/2,j+4} = \frac{1}{d_{fine}}\left(\frac{2}{9}p(i+{}^{3}/_{2}, j+{}^{9}/_{2}) + \frac{8}{9}p(i+{}^{9}/_{2}, j+{}^{9}/_{2}) - \frac{1}{9}p(i+{}^{15}/_{2}, j+{}^{9}/_{2}) - p(i+{}^{7}/_{2}, j+{}^{7}/_{2})\right)$$

7.b) Cartesian refinement

- Problem with local Cartesian grid refinement is spureous reflection at interface
  - Numerical impedance differs. Although *k dx* is the same over the whole area, α *dx* changes.



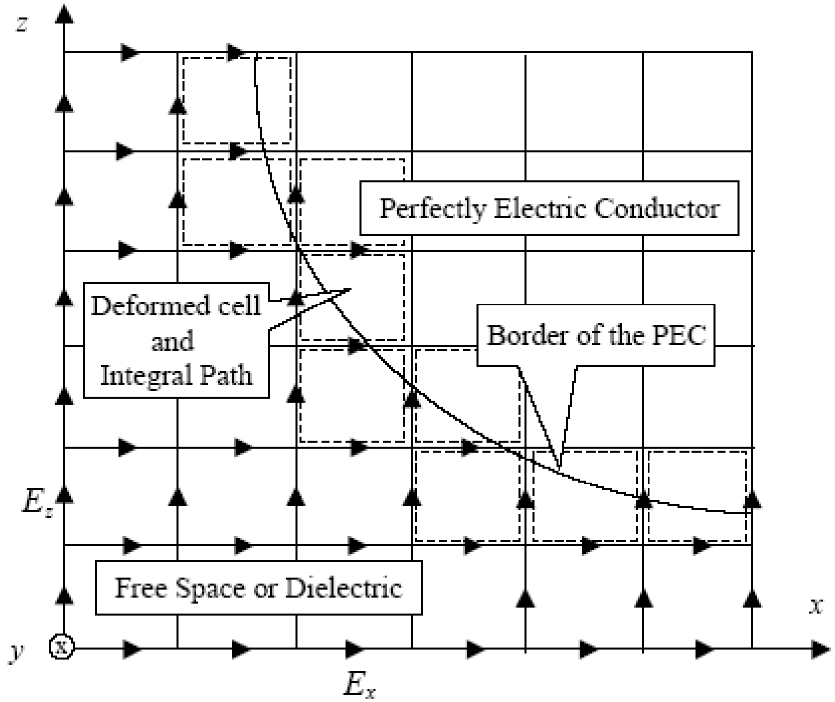
Reflection coarse to fine



Transmission coarse to fine

7.c) Non-Cartesian adaptation

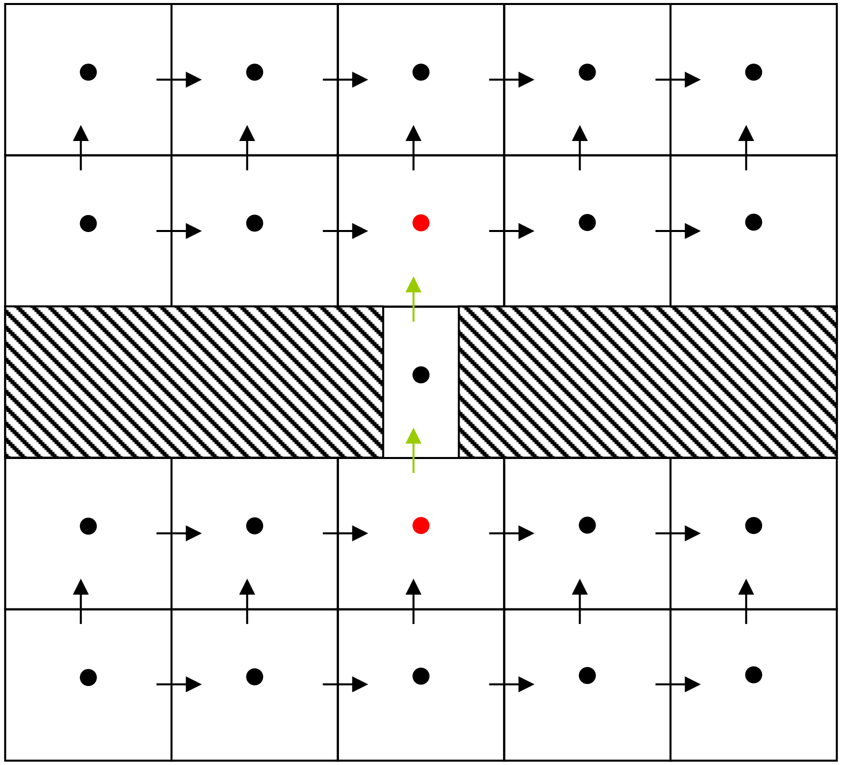
- Introduce non-Cartesian cells near the curved surface



- Non-Cartesian cells are best handled using finite volume based approach
- The approach is sometimes referred to as conformal FDTD

7.d) Small objects and openings

- Opening or object is small compared to wavelength
  - Local problem is quasi-static
  - Solve local problem (analytical or numerical) for different excitation ($p_{QS}(m)$=1, others=0)
  - Extract surface averaged $\frac{\partial p_{QS}}{\partial n}$ and p_{QS} in close by cells
  - Modified FDTD approximation



● Input for QS

↑ Modified FDTD equation

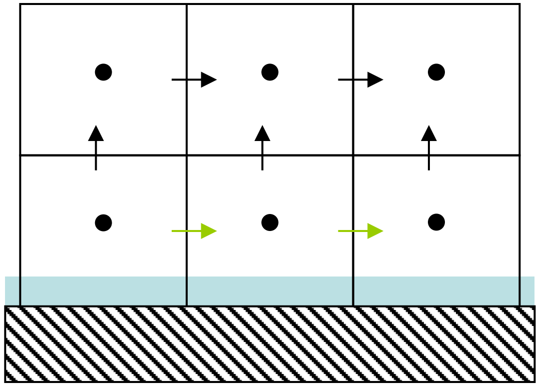
$$\left.\frac{\partial p}{\partial n}\right|_{i+1/2} \cong \frac{1}{dn}\left(p(i+1) - p(i) + \sum_m a_{m,i+1/2}\, p(m)\right)$$

$$a_{m,i+1/2} = \frac{dn}{p_{QS,m}(m)}\left(\left.\frac{\partial p_{QS,m}}{\partial n}\right|_{i+1/2} - \frac{1}{dn}\left(p_{QS,m}(i+1) - p_{QS,m}(i)\right)\right)$$

7.e) Boundary layers

- What?
  - Very local surface effect that has nevertheless a significant effect on sound propagation

$$\frac{\partial o_t}{\partial t} + \nabla p + \mu \nabla^2 o_t = 0$$



- Analytical solution in boundary layer

$$o_t = A\left(1 - e^{-n/\delta}\right) \quad \text{with} \quad \delta \approx 1/\sqrt{j\omega\nu}$$

  - Second derivative term is dominant in BL, neglect everywhere else
  - Average this term over cell and approximate considering $\delta << dn$
  - Additional term in o_t update equation $\mu \frac{o_t}{\delta dn}$
  - Note that $\sqrt{j\omega}$ must be transformed to time and discretized in time!

8. Implementation aspects

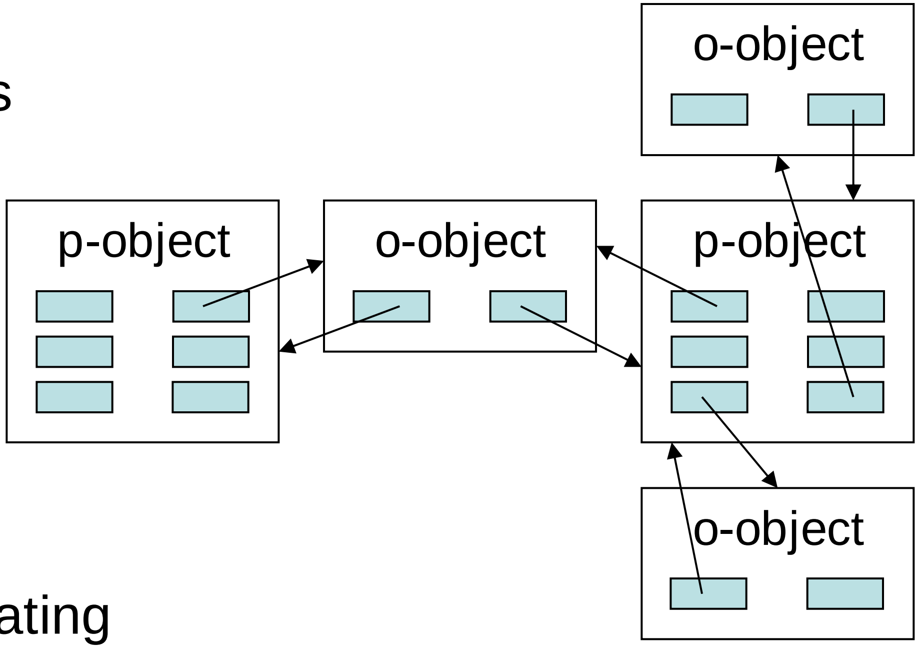
a) Matrix implementation for structured grids
b) A linked-list solution
c) Parallelization
d) Moving grids
e) Solution methods for implicit schemes

8.a) Matrix implementation for structured grids

- What?
  - p, o_x, o_y, o_z in separate matrices
  - Additional matrix for material data and choice of equation
- Pro
  - Little memory overhead
  - Fast addressing
- Contra
  - Conditional use of different update equations results in overhead
  - Cartesian bounding box may result in large number of non-used data fields if geometry contains a large number of non-propagating cells

8.b) A linked list solution

- What?
  - p/o objects linked by pointers



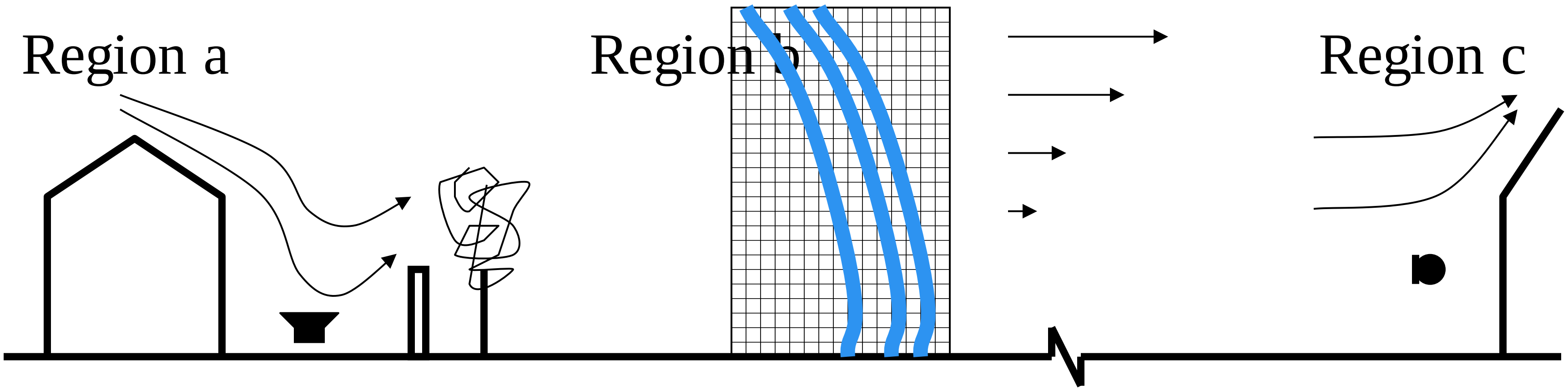
- Pro
  - Non-structured possible
  - No overhead for non-propagating
  - Different equations included naturally
- Contra
  - Memory usage

8.c) Parallelization

- Low order (staggered or not) time domain method allows for easy parallelization
- Amount of communication between CPUs is of the order n^2 in n^3 number of unknowns

8.d) Moving grids

- Memory usage may be considerably reduced
  - If pulse is short (broadband)
  - If propagation is essentially in one direction (non-resonant)
- Allocate memory only when p/o starts to rise and deallocate once the field is below a given threshold



8.e) Solution methods for implicit schemes

- Implicit schemes result in sparse matrix
- Various methods available for solving matrix equation, e.g. biconjugate gradient
- See chapter on mathematics