Numerical Simulation Methods in Geophysics, Part 13: A few more things to note

1. MGPY+MGIN

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Recap

1. The Finite Difference (FD) method
   - Poisson equation in 1D, look into 2D/3D
   - diffusion equation in 1D, time-stepping, (1D wave equation)
2. The Finite Element (FE) method
   - Poisson and diffusion equation in 1D
   - (complex) Helmholtz equation in 2D for EM problems
   - solving EM problems and computational aspects
3. Finite Volume (FV) method for advection problems

The methods

The Finite Difference method

approximates the partial derivatives by difference quotients (beware Δx and Δa)

The Finite Element method

approximates the solution through base functions in integrative sense

The Finite Volume method

approximates the solution by piecewise constant values and keeps conservation law by fluxes

Boundary conditions

Mixed boundary conditions

So far…

- Dirichlet Boundary conditions $u = u_0$
- Neumann Boundary conditions $\frac{\partial u}{\partial n} = g_B$
  for vectorial problems $\mathbf{n} \cdot \mathbf{E} = 0$ or $\boldsymbol{\nabla} \times \mathbf{E} = 0$

In general mixed, also called Robin (or impedance convective) BC

$$au + b\frac{\partial u}{\partial n} = c$$

Example DC resistivity with point source

$$\nabla \cdot \sigma \nabla u = \nabla \cdot \mathbf{j} = I\delta(\mathbf{r} - \mathbf{r}_s)$$

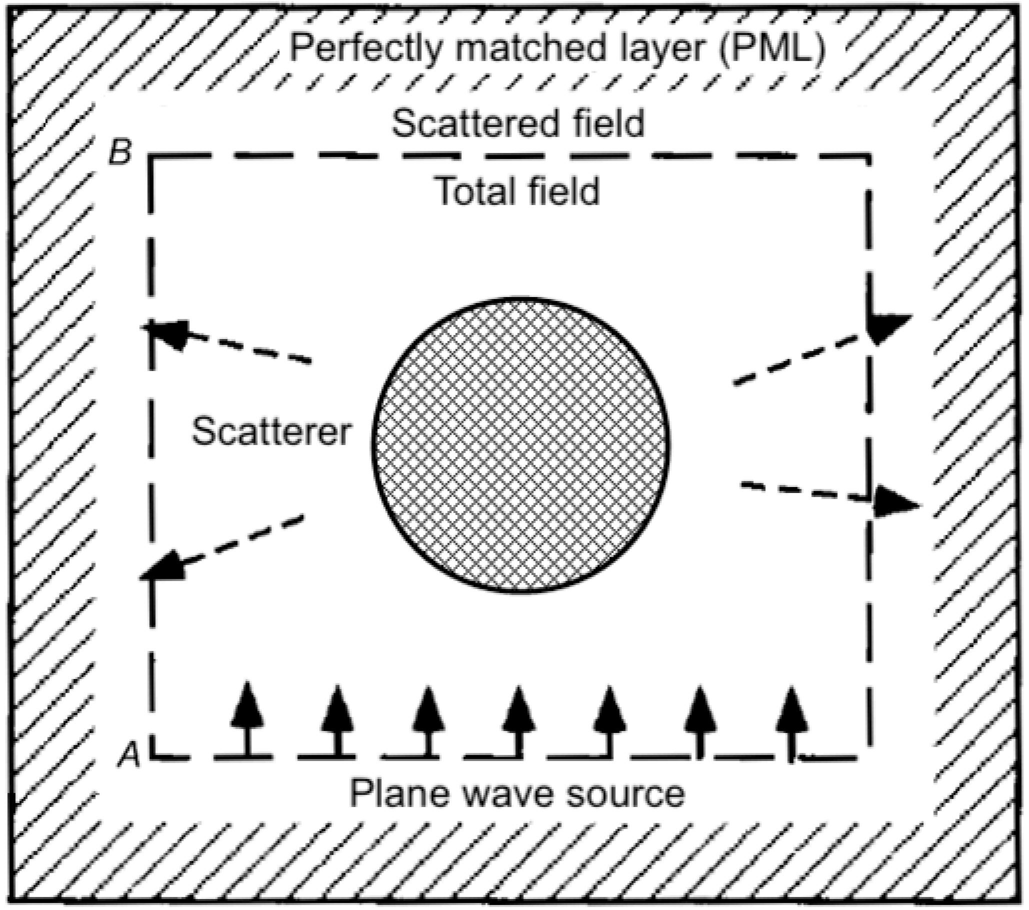
solution for homogeneous σ on surface: $u = \frac{I}{2\pi\sigma} \frac{1}{|\mathbf{r}-\mathbf{r}_s|}$

E-field $\mathbf{E} = -\frac{I}{2\pi\sigma} \frac{\mathbf{r}-\mathbf{r}_s}{|\mathbf{r}-\mathbf{r}_s|^3}$

normal direction $\mathbf{E} \cdot \mathbf{n} = -\frac{u}{|\mathbf{r}-\mathbf{r}_s|} \cos\phi$ purely geometric

$$\frac{\partial u}{\partial n} + \frac{\cos\phi}{|\mathbf{r} - \mathbf{r}_s|} = 0$$

Perfectly matched layers



$$\frac{\partial}{\partial x} \to \frac{1}{1 + i\sigma/\omega} \frac{\partial}{\partial x}$$

$$x \to x + \frac{i}{\omega} \int^{x} \sigma(x') \mathrm{d}x'$$

Absorbing boundary conditions

wave equation (e.g. in 2D)

$$\frac{\partial^2 u}{\partial t^2} - v^2 \nabla^2 u = 0$$

Fourier transform in t and y (boundary direction) $\Rightarrow \omega, k$

$$\omega^2 \hat{u} - v^2 \frac{\partial^2 \hat{u}}{\partial x^2} + v^2 k^2 \hat{u} = 0$$

ordinary DE with solution $\hat{u} = \sum a_i e^{\lambda x}$ with $\lambda^2 = k^2 - \omega^2 / v^2$

Modern methods

Solution in wavenumber domain

Fourier transform of 3D problem into wavenumbers

$$\hat{F}(k_x, y, z) = \int_{-\infty}^{\infty} F(x, y, z) e^{-\imath k_x x} \mathrm{d}x$$

partial derivative $\frac{\partial^2 \hat{F}}{\partial x^2} = k_x^2 \frac{\partial^2 F}{\partial x^2}$

Poisson equation $\nabla^2_{3D} u = 0 \Rightarrow$ Helmholtz equation $\nabla^2_{3D} \hat{u} - k_x^2 \hat{u} = 0$
$\Rightarrow$ solve many 2D problems & get solution by inverse Fourier transform

Spectral element method

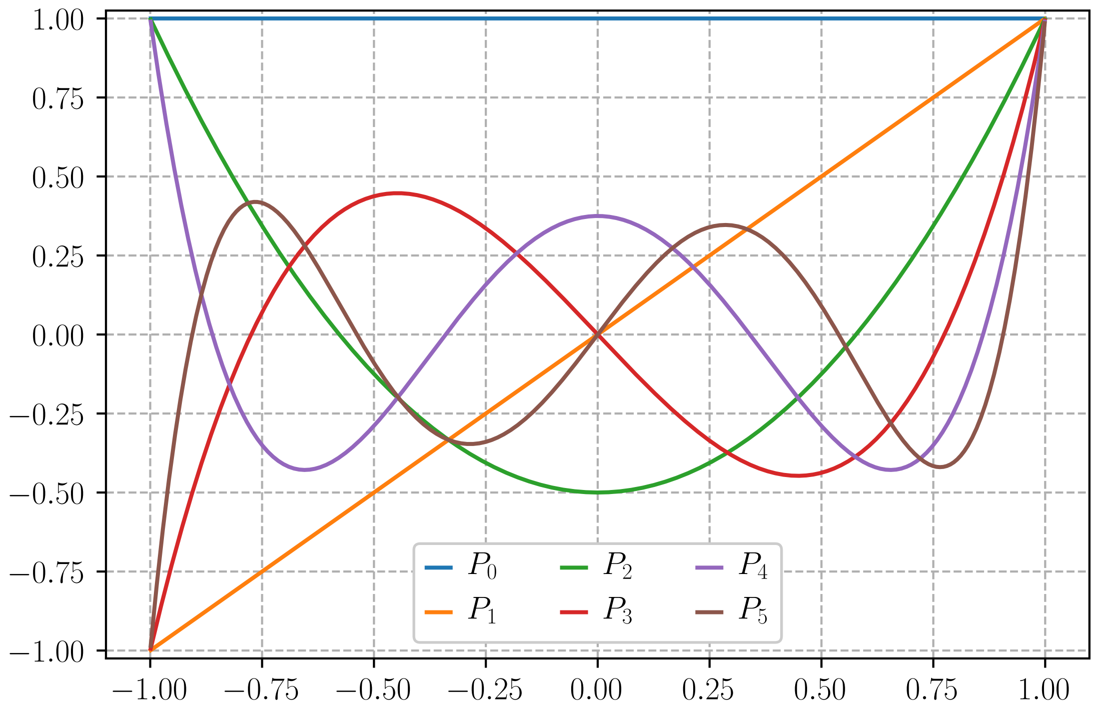
typically used for global wave phenomena

$$u = \sum u_i \phi_i(\mathcal{P}r)$$

ϕ Lagrangian polynoms

$$l_i^N = \prod_k^N \frac{\xi - \xi_k}{\xi_i - \xi_k}$$

or Chebychev polynoms



First six Lagrangian polynomials

Discontinuous Galerkin method

typical for hyperbolic problems

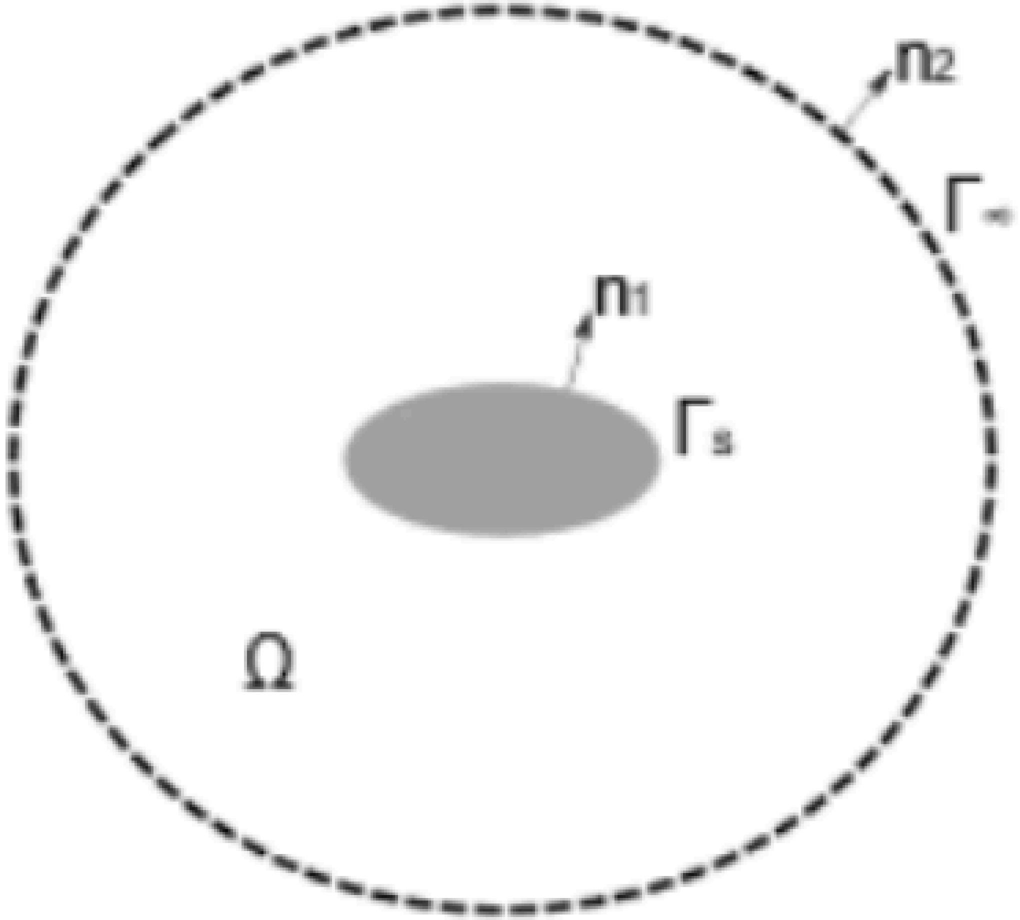
weak form of wave equation with fluxes (FV)

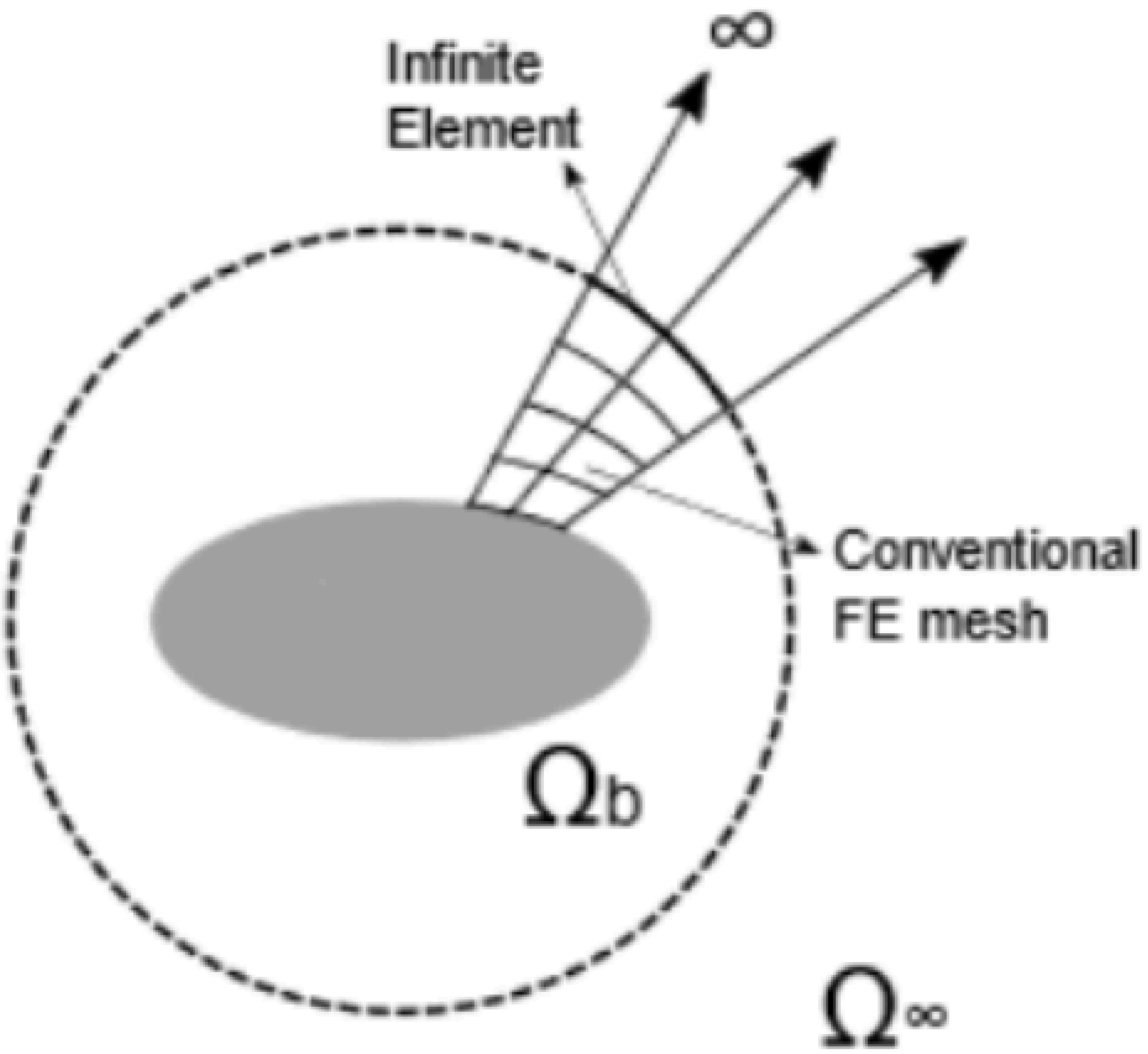
$$M\partial_t q(t) - A^T q(t) = -F(a, q(t))$$

$$\Rightarrow \partial_t q = \mathbf{M}^{-1}(A^T q(t) - F(a, q(t)))$$

locally for each element & communication through fluxes (like in FV)

Infinite Elements





Meshless modelling

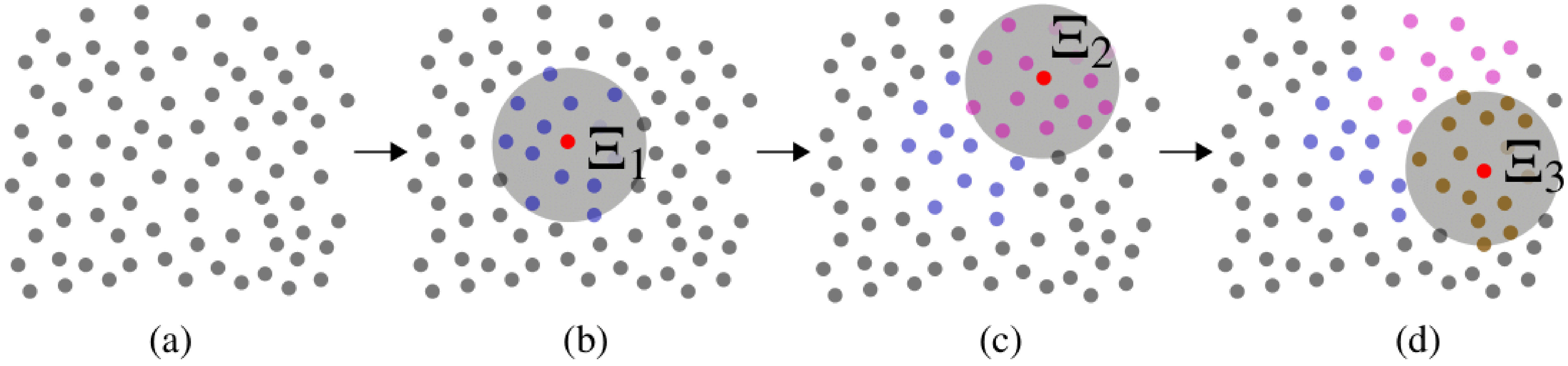


Figure 3.5: Overview of meshless computational scheme. From a set of points (a) local subsets (stencils) Ξ_i $i = \{1, 2, 3\}$ are selected as displayed in (b) to (c) to construct a meshless approximation.

Meshless divergence operator (Wittke, 2017)

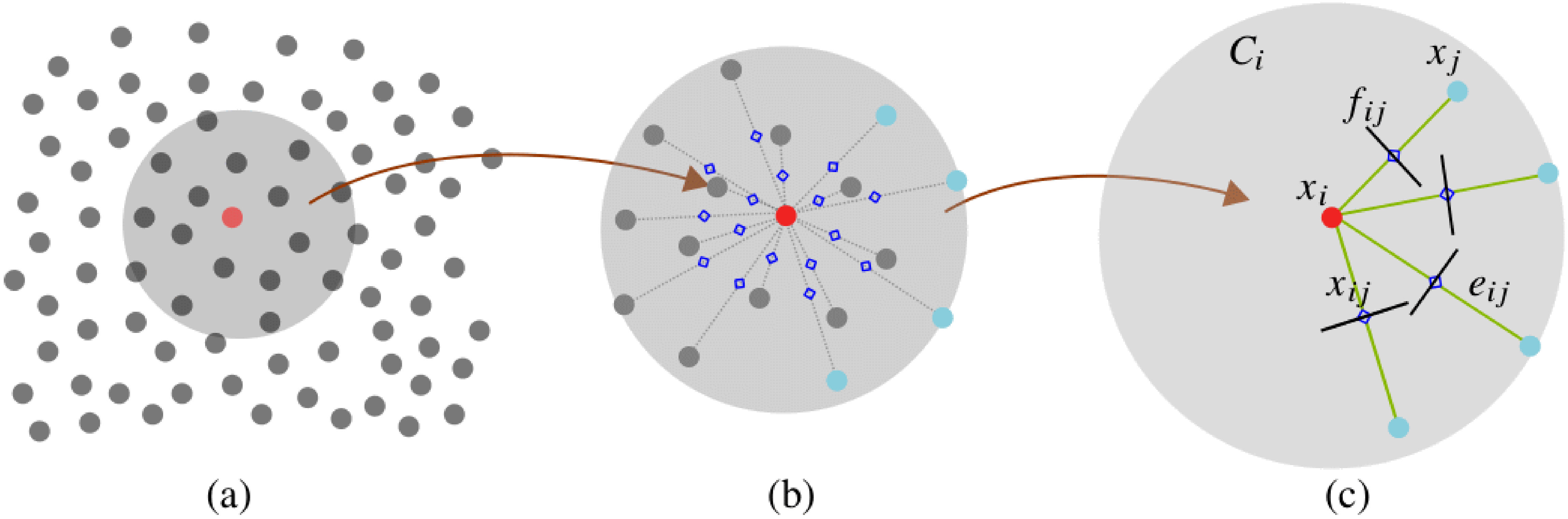


Figure 3.6: Stencil-wise construction of a local primal-dual grid complex. (a) Selecting enough points to form a stencil in a predefined neighbourhood. (b) Definition of midpoints (blue diamonds) from the central point to all other points. (c) Definition of the primal edges e_{ij} and dual faces f_{ij} inside a dual cell C_i from the definition of midpoints x_{ij}.

Error estimation and mesh refinement

- get idea of accuracy of the solution
- refinement of cells with high error (e.g. large gradients)
- comparison between successive refinement solutions

Error estimation (residual-based)

Poisson problem $-\nabla^2 = f$ with bilinear form $a(u, v) = \int \boldsymbol{\nabla} u \boldsymbol{\nabla} v \mathrm{d}\Omega$

finite-dimensional function space V_h: $a(u_h, v_h) = l(v_h)$

estimate error e_h in bilinear form $a(e_h, v) = a(u, v) - a(u_h, v)$

residual $R = f + \nabla^2 u_h$ leads to $a(e_h, v) = \sum_c \int_{\Omega_c} R v \mathrm{d}\Omega_c$

Error estimation (recovery-based)

gradients across element boundaries tend to be discontinuous

compare original (unsmoothed) gradient of the solution with improved

$$(E_h)^2 = \int |M(u_h) - \boldsymbol{\nabla} u_h|^2 \mathrm{d}\Omega$$

M obtained by smoothing over patch of elements around each element

Goal-oriented mesh refinement

primal and dual (adjoint) problem (with receiver as hypothetical source)

inner product of solutions

$$\Phi_{lmn} = \int_{c_n} \mathbf{F}^l \mathbf{F}^m \mathrm{d}\Omega_n$$