Multiscale modelling of materials with periodic micro-structures

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The material presented is taken from a dissertation written at UT-Austin under the supervision of Ivo Babuška and Gregory Rodin.

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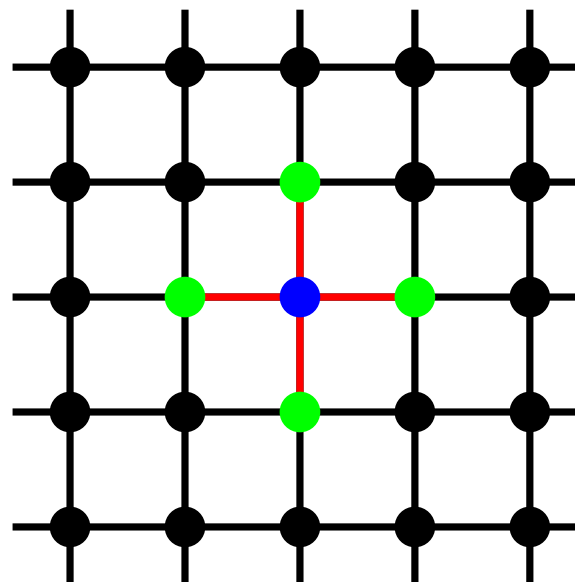
A MODEL PROBLEM

Consider heat conduction on the simple square lattice $\mathbb{Z}^2$. Let $\boldsymbol{u}(m)$ denote the temperature of node $m \in \mathbb{Z}^2$ and let $\boldsymbol{f}(m)$ denote an external heat source. Then the equilibrium equations read

$$[\boldsymbol{Au}](m) = \boldsymbol{f}(m), \quad \forall\, m \in \mathbb{Z}^2,$$

where

$$[\boldsymbol{Au}](m) = 4\boldsymbol{u}(m_1, m_2) - \boldsymbol{u}(m_1 - 1, m_2) - \boldsymbol{u}(m_1 + 1, m_2)$$
$$- \boldsymbol{u}(m_1, m_2 - 1) - \boldsymbol{u}(m_1, m_2 + 1).$$

The operator $\boldsymbol{A}$ is known as the *discrete Laplace operator*.
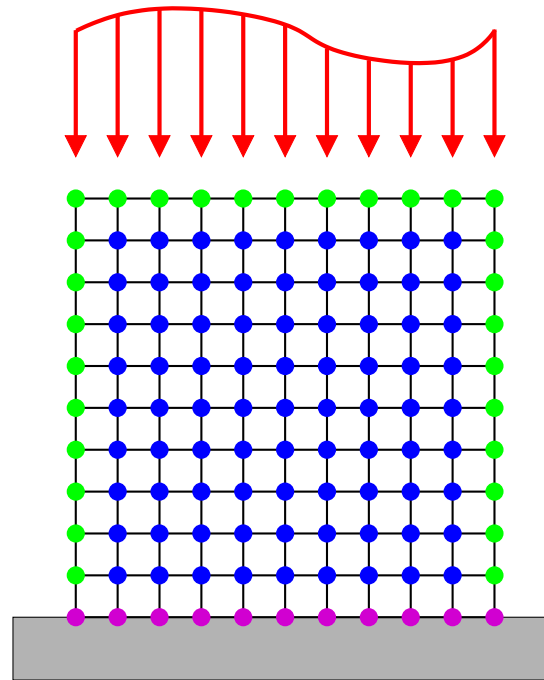
Boundary conditions:

Collect the N nodes in $\Omega \subset \mathbb{Z}^2$.
Split $\Omega = \Omega_\mathrm{i} \cup \Gamma_\mathrm{D} \cup \Gamma_\mathrm{N}$, where

Ω_i are the interior nodes,

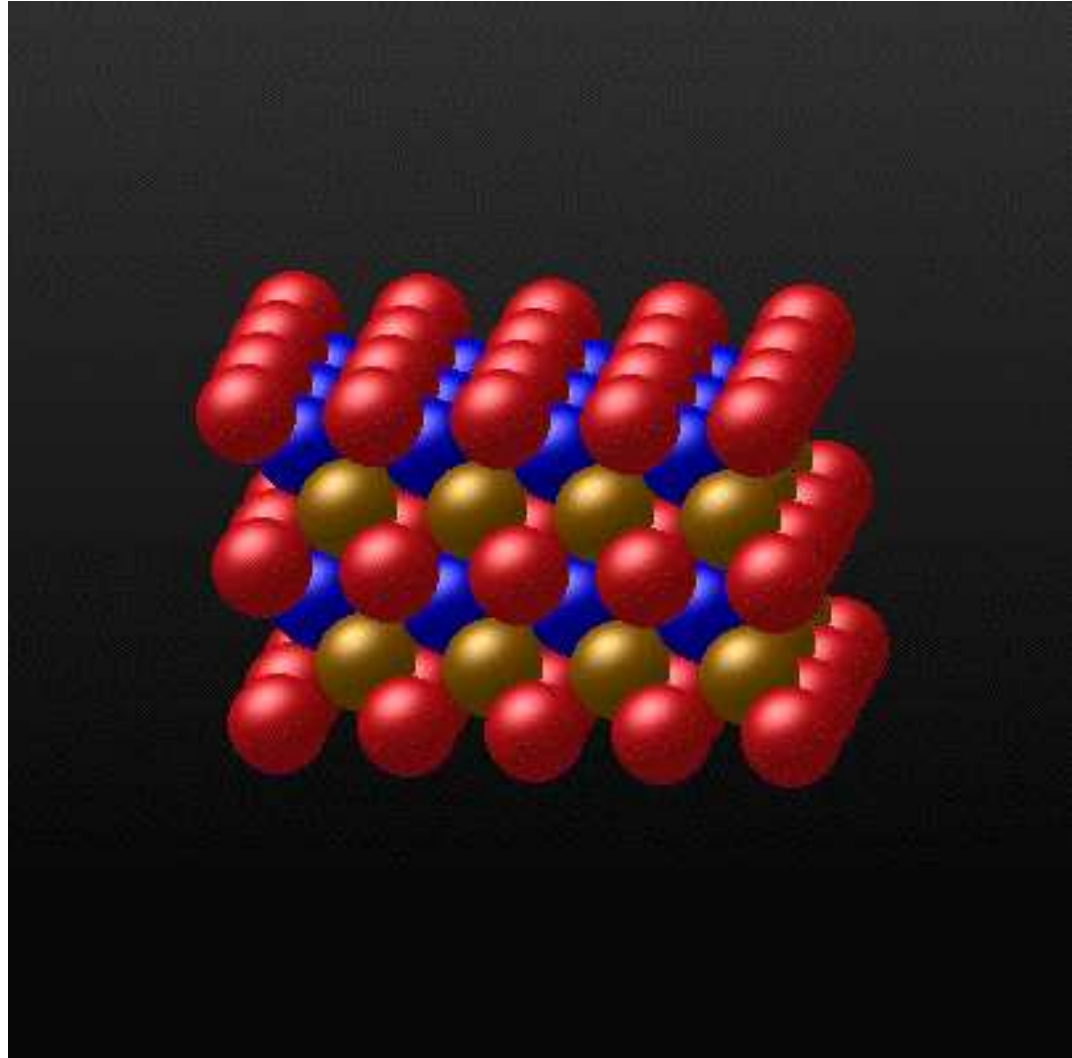Γ_D is the Dirichlet boundary,

Γ_N is the Neumann boundary.

We can now formulate the discrete boundary value problem

$$\begin{cases} \boldsymbol{Au} = \boldsymbol{f}, & \text{on } \Omega_\mathrm{i}, \\ \boldsymbol{u} = \boldsymbol{g}, & \text{on } \Gamma_\mathrm{D}, \\ \partial_\nu \boldsymbol{u} = \boldsymbol{h}, & \text{on } \Gamma_\mathrm{N}, \end{cases}$$

where $\boldsymbol{A}$ is the discrete Laplace operator.

Similar equations model linear interactions between atoms in a crystal.

For the problems considered; traditional homogenization techniques do not perform very well.

Concentrated loads are common.

It is important to capture the mechanics at boundaries and corners.

The most interesting cases involve lattice imperfections, modelling buckling of bars, etc.

In other words, there is typically no separation of length-scales.
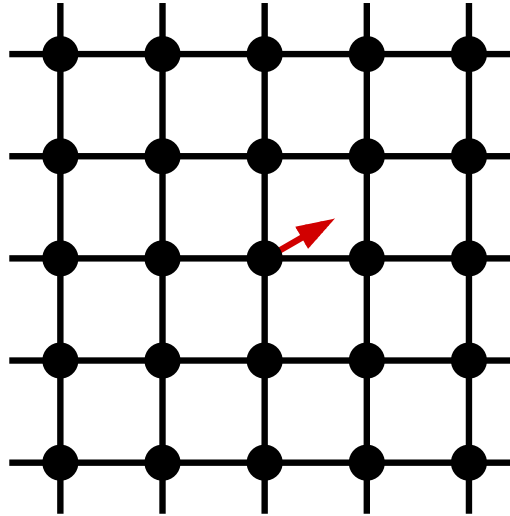
Our solution:

1. Derive a fundamental solution for an infinite lattice.

2. For finite structures, use the fundamental solution to rewrite the equilibrium equations as an equation on the boundary.
   This is an exact procedure, no approximation is involved.

3. If the boundary equations involve too many degrees of freedom, use asymptotic expansions in the fundamental solution.

Earlier work (an emphatically non-complete bibliography!):

- *Fourier methods for analyzing difference equations.*
  Babuška 1970
  Fix and Strang 1973, Stefan 1976, <u>Saltzer 1958</u>, Duffin 1953.

- *Homogenization*
  Babuška 1975, 1976, 1977, 1979, 2000,...
  Berlyand and Kolpakov 2001, Blanc, LeBris and Lions 2002,
  Cioranescu and Saint Jean Paulin 1999, Gibson and Ashby 1989,
  Lakes 1991, Panasenko 1998, Vogelius 1991.

- *Analysis of lattice structures*
  Babuška and Morgan 1991, Babuška and Sauter 2004
  Evans, Hutchinson and Ashby 1998, Friesecke and Theil 2002, Noor
  1998, Ostoja-Starzewski 2002, Schwab and Matache 2000.

- *Fast summation methods*
  Greengard and Rokhlin 1987.

We apply a heat source of unit strength at the origin of the lattice and calculate the resulting equilibrium temperature. We label this solution $\boldsymbol{G} = \boldsymbol{G}(m)$, for $m \in \mathbb{Z}^2$. Then, $\boldsymbol{G}$ satisfies the equation

$$[\boldsymbol{AG}](m) = \delta(m), \qquad m \in \mathbb{Z}^2,$$

where δ is the Dirac delta function,

$$\delta(m) = \begin{cases} 1 & \text{for } m = 0, \\ 0 & \text{for } m \in \mathbb{Z}^2 \backslash \{0\}. \end{cases}$$

0

From the previous slide, we have the equilibrium equation

$$(1) \qquad [\boldsymbol{AG}](m) = \delta(m), \qquad m \in \mathbb{Z}^2.$$

The discrete Fourier transform is defined by

$$\tilde{\boldsymbol{u}}(\xi) = [\boldsymbol{Fu}](\xi) = \sum_{m \in \mathbb{Z}^2} e^{\mathbf{i}m \cdot \xi} \boldsymbol{u}(m), \qquad \text{for } \xi \in (-\pi, \pi)^2.$$

Fourier transforming (1) we obtain the formula

$$(2) \qquad \sigma(\xi)\tilde{\boldsymbol{G}}(\xi) = 1, \qquad \text{for } \xi \in (-\pi, \pi)^2,$$

where $\sigma(\xi)$ is the *symbol* of $\boldsymbol{A}$,

$$\sigma(\xi) = 4 - e^{\mathbf{i}\xi_1} - e^{-\mathbf{i}\xi_1} - e^{\mathbf{i}\xi_2} - e^{-\mathbf{i}\xi_2} = 4 \left(\sin^2 \frac{\xi_1}{2} + \sin^2 \frac{\xi_2}{2} \right).$$

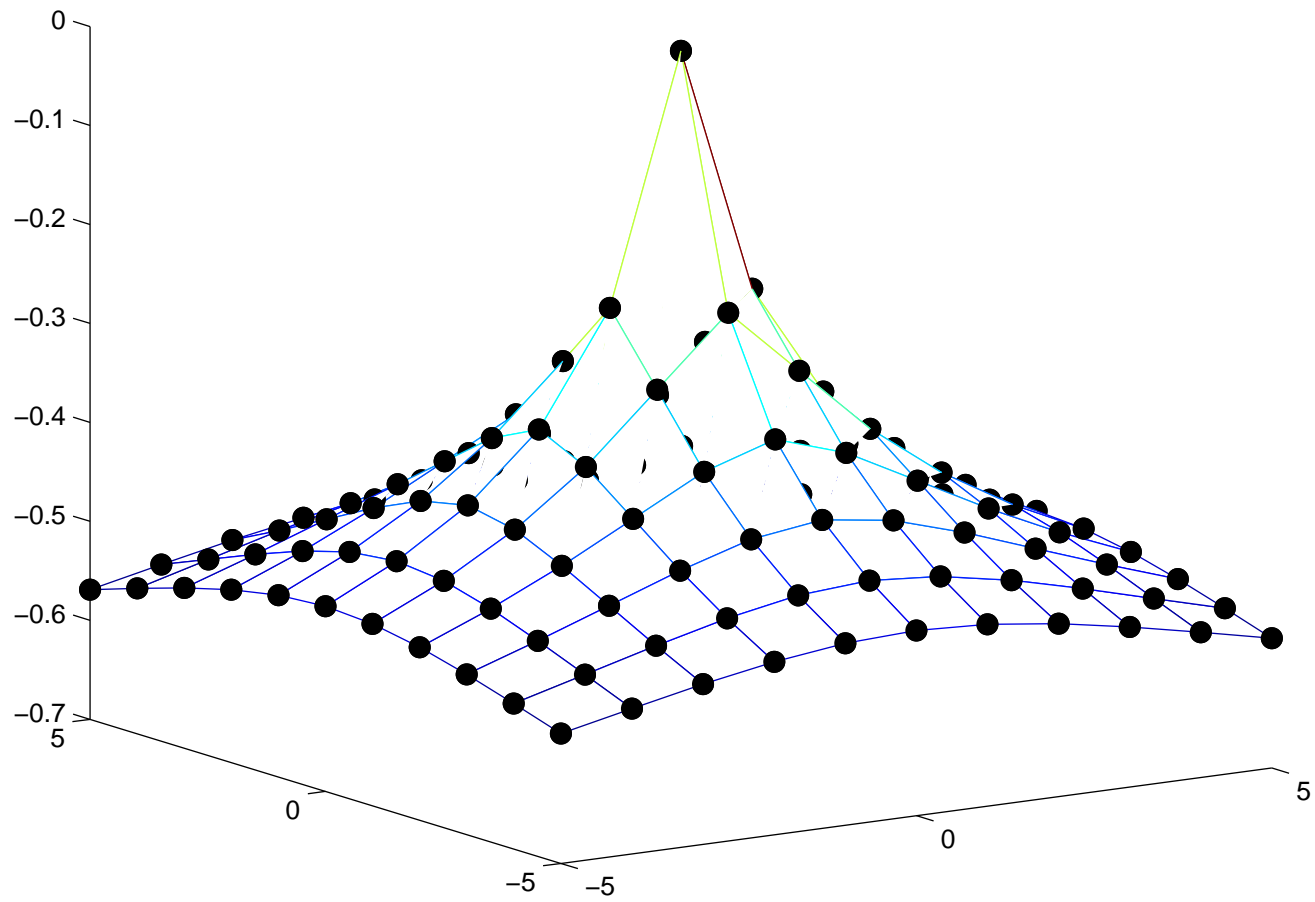From (2), we get $\tilde{\boldsymbol{G}} = 1/\sigma$, and then

$$\boldsymbol{G}(m) = \frac{1}{(2\pi)^2} \int_{(-\pi,\pi)^2} e^{-\mathbf{i}\xi \cdot m} \tilde{G}(\xi) \, d\xi = \frac{1}{(2\pi)^2} \int_{(-\pi,\pi)^2} e^{-\mathbf{i}\xi \cdot m} \frac{1}{\sigma(\xi)} \, d\xi.$$

<u>MEA CULPA</u>

We have cheated, $|\xi|^{-2}$ is not integrable in two dimensions ...

Without going into details, we simply assert that the following regularization works:

$$\boldsymbol{G}(m) = \frac{1}{(2\pi)^2} \int_{(-\pi,\pi)^2} \frac{e^{-\mathbf{i}m\cdot\xi} - 1}{\sigma(\xi)} \, d\xi.$$

Plot of the lattice Green's function.

$$G(m) = \frac{1}{(2\pi)^2} \int_{(-\pi, \pi)^2} \frac{e^{-im\cdot\xi} - 1}{\sigma(\xi)} \, d\xi$$

The singularity of $\sigma(\xi)^{-1}$ is captured by the expansion

$$\frac{1}{\sigma(\xi)} = \frac{1}{|\xi|^2} + \frac{1}{12} \frac{\xi_1^4 + \xi_2^4}{|\xi|^4} + O(|\xi|^2).$$

We then expect that

$$G(m) \approx \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left[\frac{e^{-im\cdot\xi} - 1}{|\xi|^2} + e^{-im\cdot\xi} \frac{1}{12} \frac{\xi_1^4 + \xi_2^4}{|\xi|^4} \right] d\xi =: G_1(m),$$

which evaluates to (for $m \neq 0$)

$$G_1(m) = -\frac{1}{2\pi} \left(\log|m| + \gamma + \frac{\log 8}{3} \right) + \frac{1}{24\pi} \frac{m_1^4 - 6m_1^2 m_2^2 + m_2^4}{|m|^6}.$$
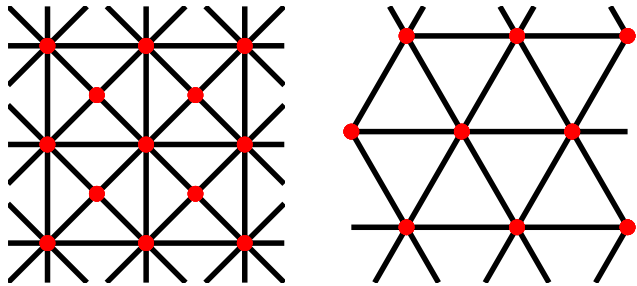
Remarks on the lattice Green's function $\boldsymbol{G}(m)$:

- $\boldsymbol{G}(m)$ is a matrix for multi-atomic lattices.

- The asymptotic expansion can be computed automatically using symbolic algebra software.

- Homogenized equations can directly be read off from the asymptotic expansion.

- $\boldsymbol{G}(m)$ captures the close-range behavior *exactly*.

Mechanical lattices of two types. (Much more interesting!)

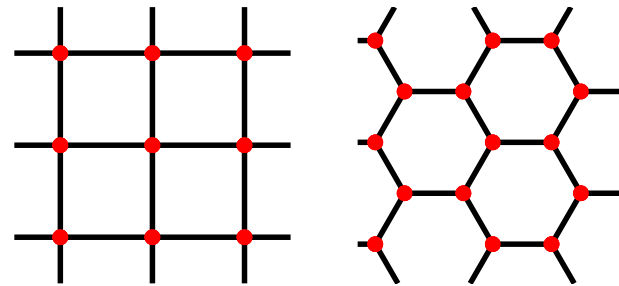| Truss Lattices	Frame Lattices
Strength from **axial** stiffness.	Strength from **bending** stiffness.
Symbol is always a matrix:	Symbol is always a matrix:
2 degrees of freedom per node.	3 degrees of freedom per node.
Asymptotics: Classical elasticity.	Asymptotics: Cosserat elasticity.
	Typically very anisotropic.

Asymptotic expansions can again be derived automatically.

Everything works ... the theory for all this is fairly well understood.
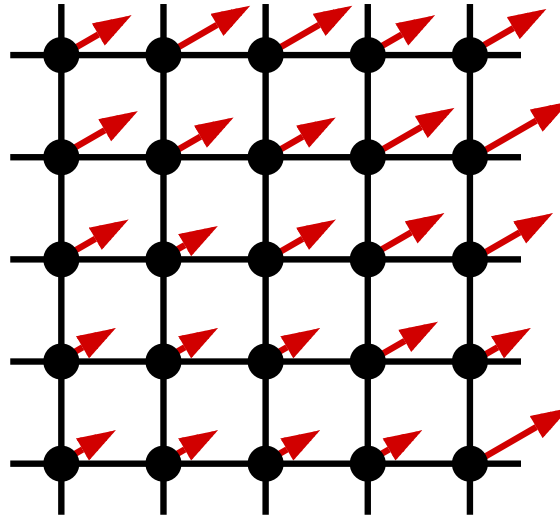
The equilibrium equation reads

$$[\boldsymbol{Au}](m) = \boldsymbol{f}(m), \qquad m \in \mathbb{Z}^d$$

The solution is simply a convolution between $\boldsymbol{f}$ and $\boldsymbol{G}$;

$$\boldsymbol{u}(m) = [\boldsymbol{G} * \boldsymbol{f}](m) = \sum_{n \in \mathbb{Z}^2} \boldsymbol{G}(m - n)\boldsymbol{f}(n).$$

Recall that there is no explicit formula for the fundamental solution $\boldsymbol{G}$! However, we know the asymptotic expansion of $\boldsymbol{G}$, and can use this in combination with fast summation methods similar to the FMM.

We consider a Dirichlet problem
on the L-shaped domain

$$\boldsymbol{A}\boldsymbol{u} = 0, \qquad \text{on } \Omega_{\mathrm{i}},$$

$$\boldsymbol{u} = \boldsymbol{g}, \qquad \text{on } \Gamma.$$
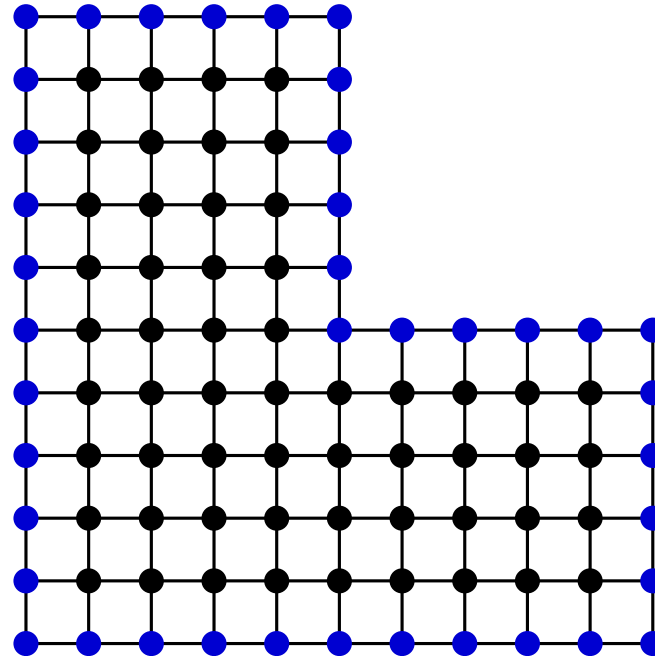
Make a "double layer Ansatz":

$$\boldsymbol{u}(m) = \sum_{n \in \Gamma} \partial_{\nu_n} \boldsymbol{G}(m - n)\phi(n) =: [K_{\mathrm{D}}\,\phi](m),$$

where $\partial_{\nu_n} \boldsymbol{G}(m - n)$ is a discrete analogue of the double layer kernel. Then

(3) $$\sum_{n \in \Gamma} \partial_{\nu_n} \boldsymbol{G}(m - n)\phi(n) = \boldsymbol{g}(m), \qquad \forall\, m \in \Gamma.$$
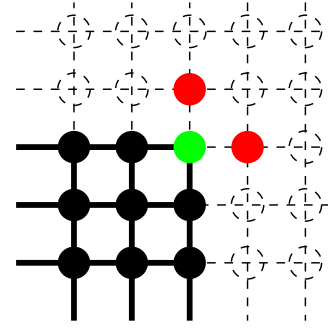
Numerical experiments indicate that (3) is very well-conditioned.
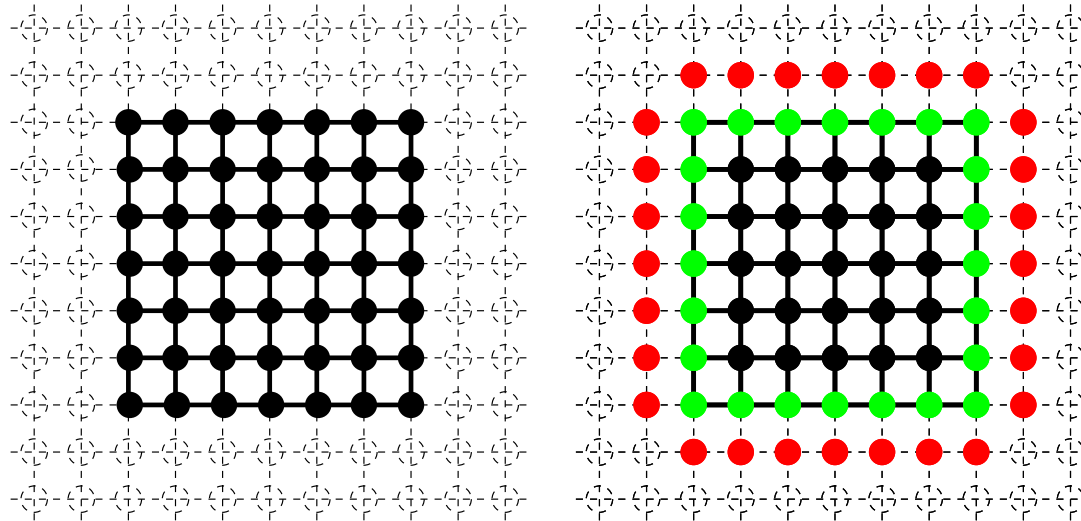(We have no proofs.)

∂_ν is an external difference operator: given a boundary node n, let $\mathbb{D}_n \subset \Omega^c$ be the set of nodes that connect to n, then
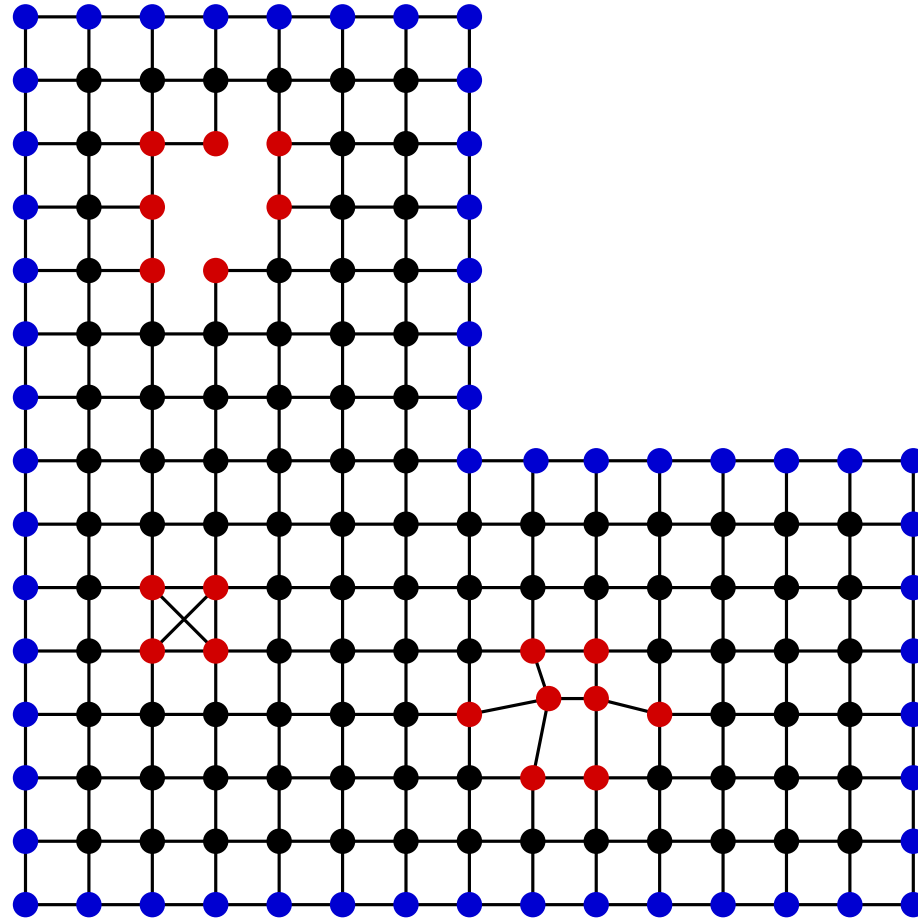
$$[\partial_\nu \psi](n) = \sum_{k \in \mathbb{D}_n} (\psi(k) - \psi(n)).$$

Thus, the ansatz corresponds to placing charges of opposite signs on the red and the green nodes in the figure below

As long as the sites of irregularities do not dominate the problem, they can easily be included in the set of point on which the "boundary equation" is defined.

Main point: The method of reformulating a linear PDE as a boundary integral equation can be applied to problems with periodic lattice micro-structures.

Benefits:

- Model simplification does not rely on separation of length-scales.
- Boundaries and concentrated loads cause no loss of accuracy.
- The equations to be solved are inherently well-conditioned.
- Homogenization of integral operator rather than differential operator.
- Full error control. Errors on the order of 10^{-10} are easily achievable.

Possible extensions:

- Problems with *continuum* periodic micro-structure.

Principal limitations:

- Linear problems.
- Periodic micro-structures. (Localized imperfections are OK.)