Summation rules for higher order Quasi-continuum methods

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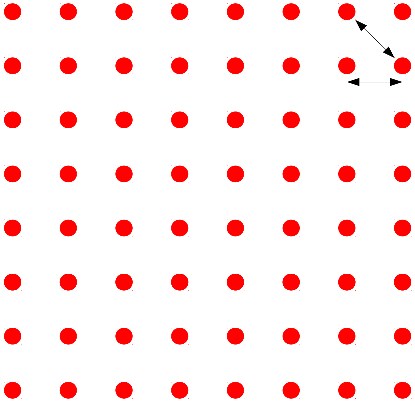
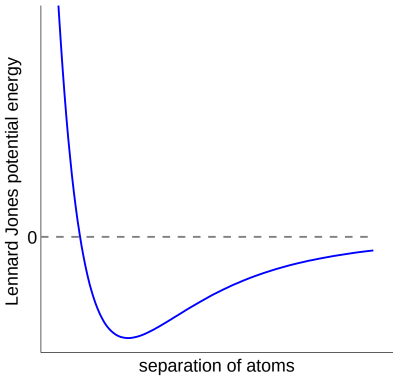
Overview

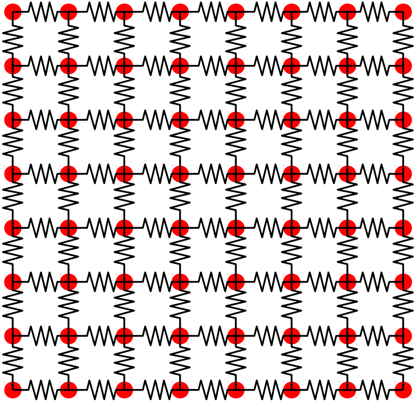
1. Lattice models
   - Atomistic lattice models
   - Structural lattice models

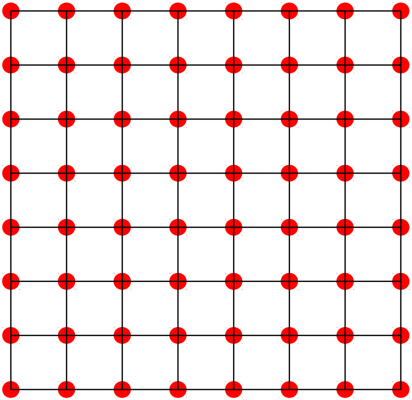
2. The Quasi-continuum method
   - Formulation
   - Approximations
   - Summation rules

3. Results




Lennard Jones potential energy
0
separation of atoms





Lattice models comprising springs or beams have been used to model

- atomistic crystalline materials
- fibrous materials
- collagen networks
- heterogenous materials

Quasi-continuum method:

aims to reduce the computational cost of calculations associated with lattice models

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For displacements and rotations,

$$\mathbf{a}^{\mathrm{T}} = \{u_i, v_i, w_i, \theta_i^x, \theta_i^y, \theta_i^z\}_{i=1}^{nNodes} \ ,$$

we minimise the potential energy of the system:

$$\arg\min(E_{\mathrm{int}}(\mathbf{a}) - \mathbf{f_{ext}} \cdot \mathbf{a}), \quad \text{where} \quad E_{\mathrm{int}} = \sum_{j=1}^{beams} E_j$$

$$\left[\frac{\partial^2 E_{\mathrm{int}}}{\partial \mathbf{a}^2}\right] \mathbf{a} = \mathbf{f}_{\mathrm{ext}}$$

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Efficiencies made in the coarse region:

1. "interpolation": number of degrees of freedom are reduced by introducing representative lattice nodes or "rep-atoms"

$$\mathbf{a_r}^{\mathrm{T}} = \{u_i, v_i, w_i, \theta_i^x, \theta_i^y, \theta_i^z\}_{i=1}^{rNodes} \quad ,$$

2. "summation rule": find representative interactions or sampling beams
   - determine which beams will be used in the summation
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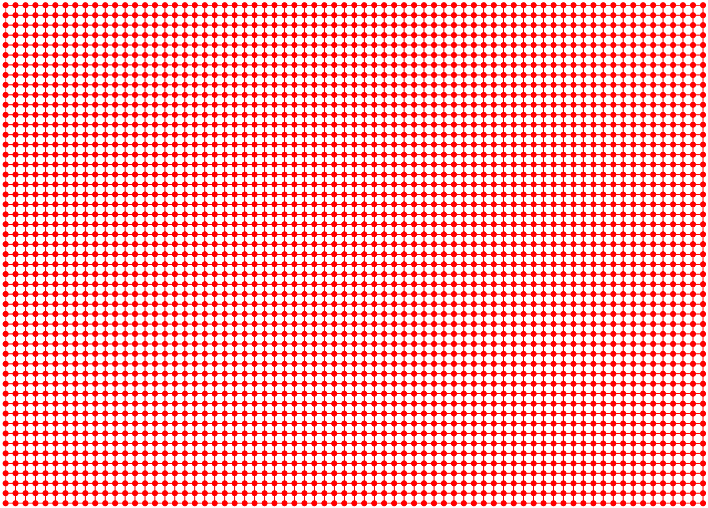

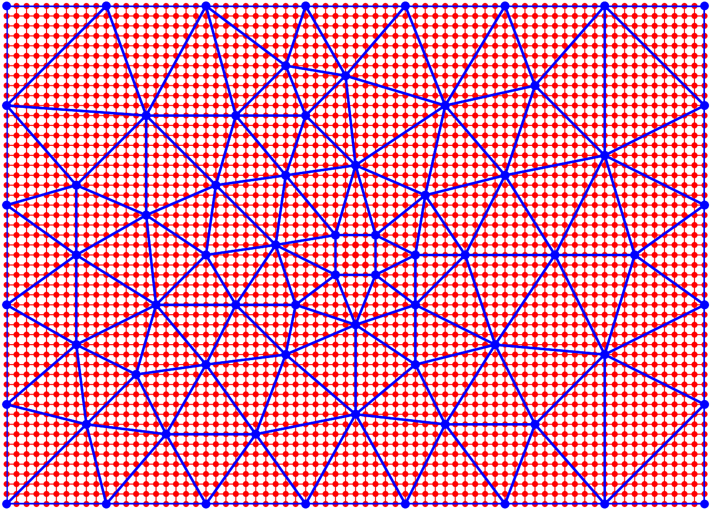

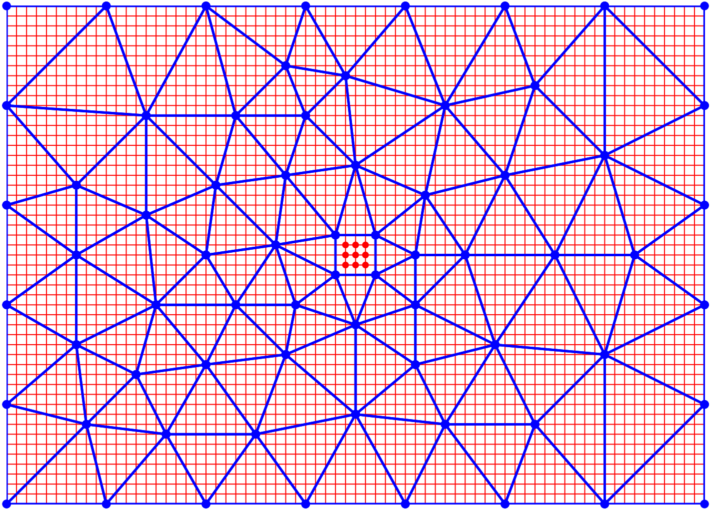

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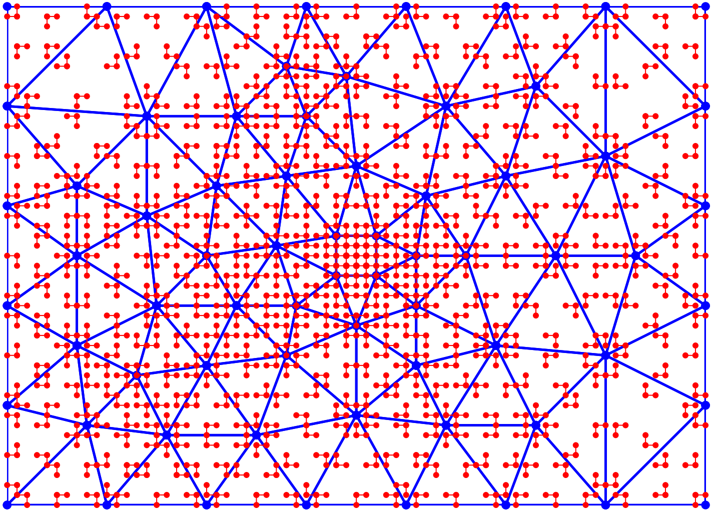

Advantages of QC

- lattice defects can be modelled accurately (in the fully resolved region)
- no continuum model is required in the coarse region, as the approximation is based on the lattice model itself

Disadvantage of QC

- irregular lattice models are still challenging

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Summation rules - guided by Gaussian quadrature rules.

Three rules:

- closest summation rule (implemented in Beex *et. al.* 2014)
- mid-beam rules
  - non-local
  - local

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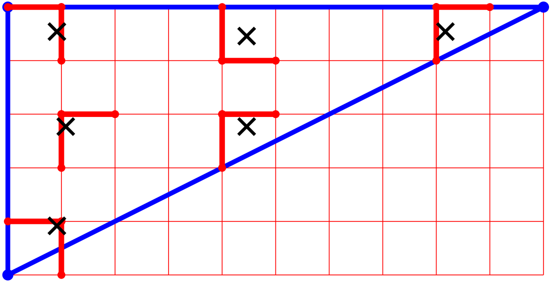
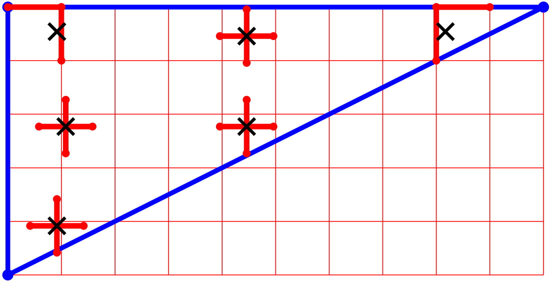
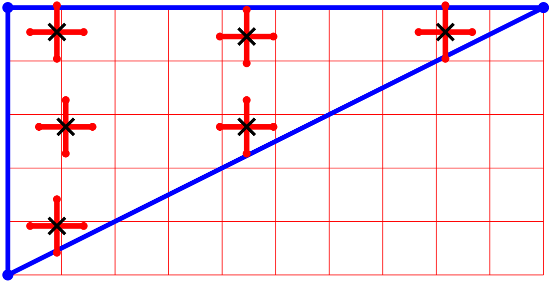
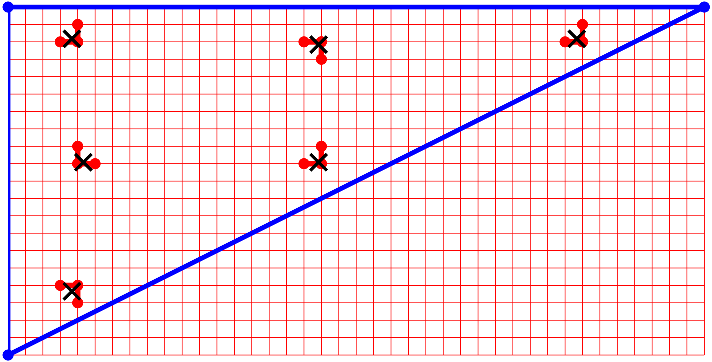


Quasi-continuum method
Mid-beam summation rule (closest, non-local)

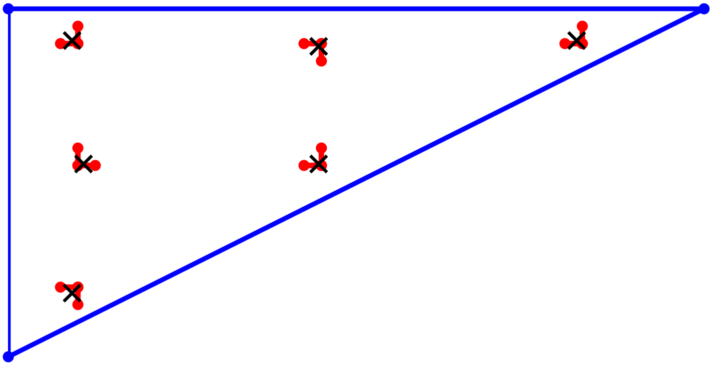


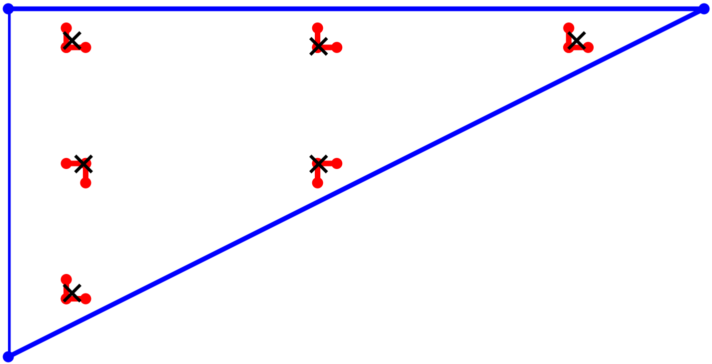
Quasi-continuum method
Mid-beam summation rule (local)

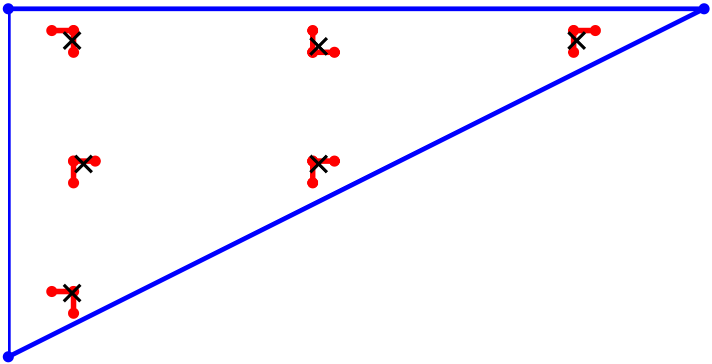


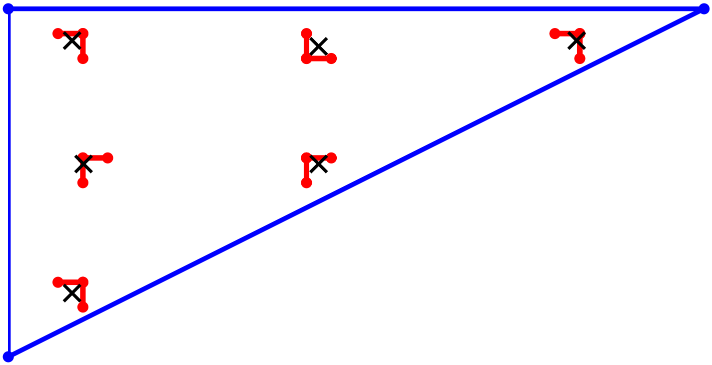


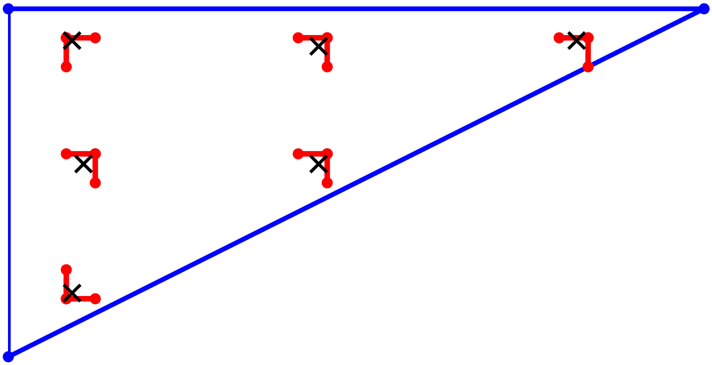
Quasi-continuum method
Closest summation rule

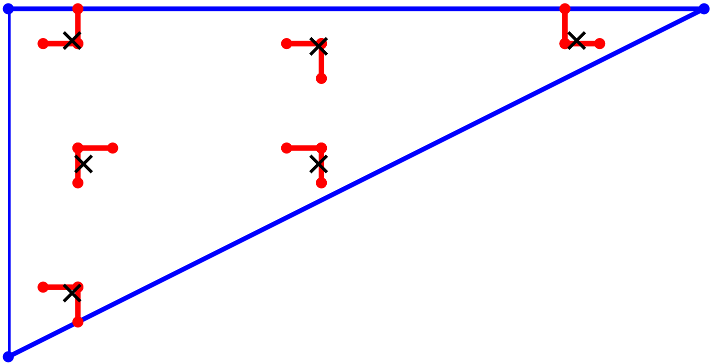


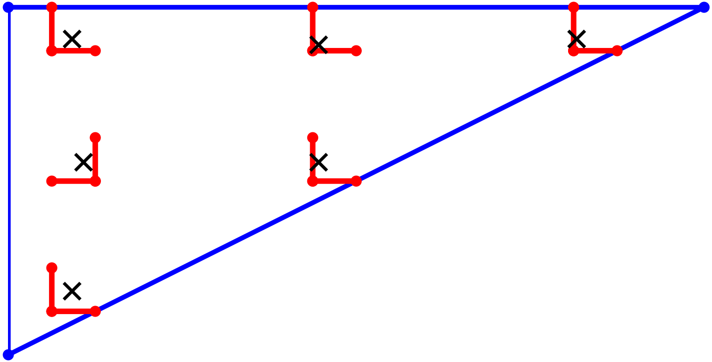


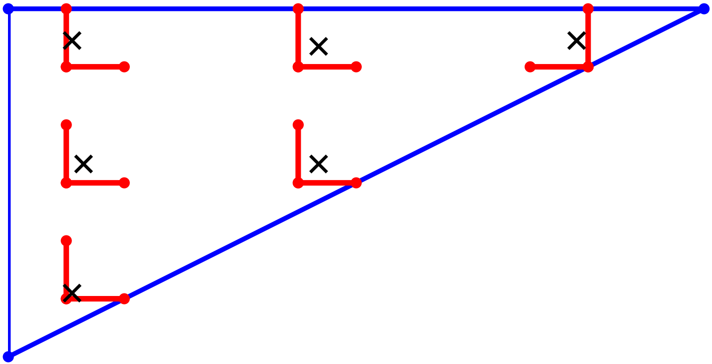


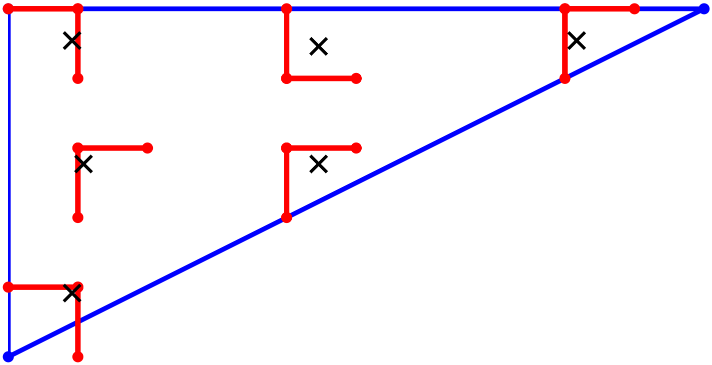


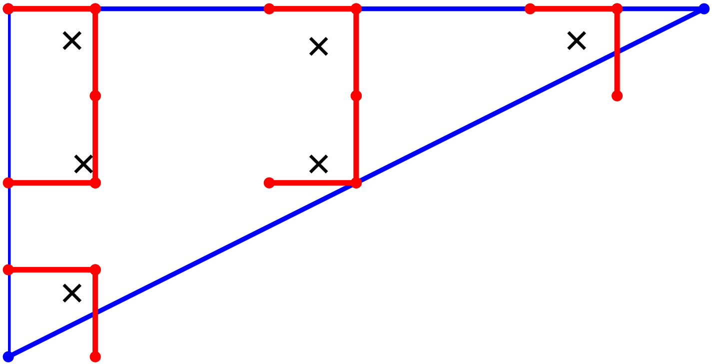


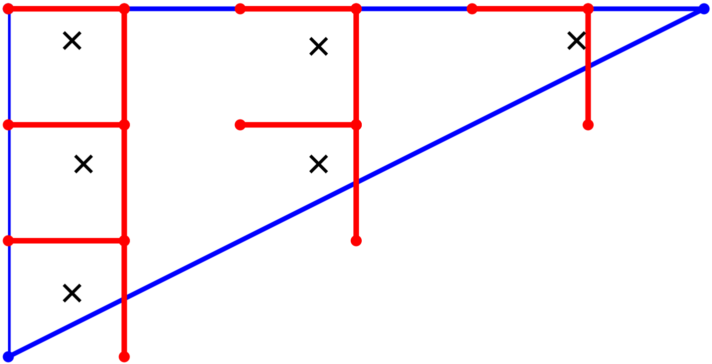


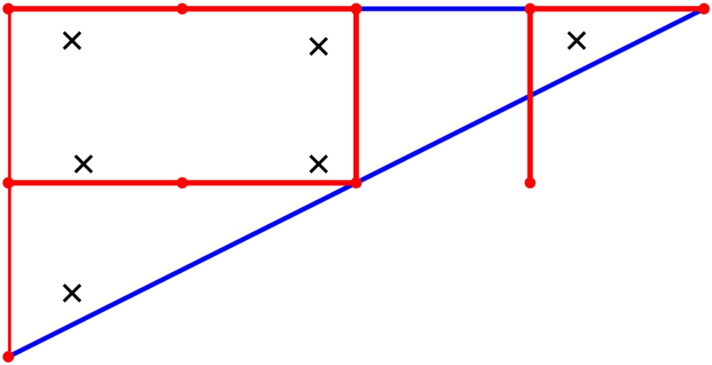


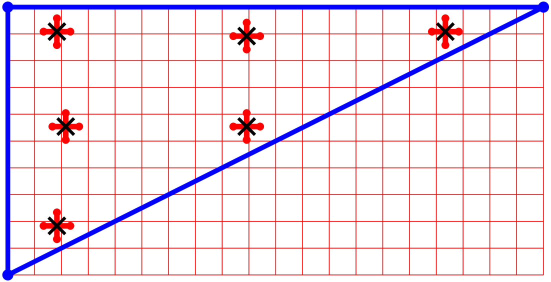


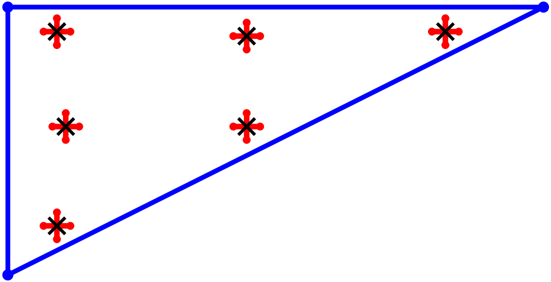


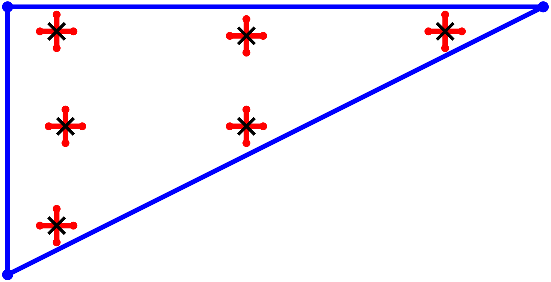


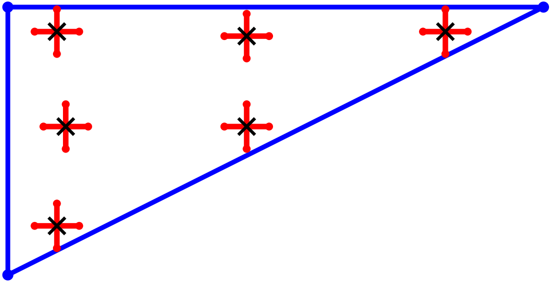




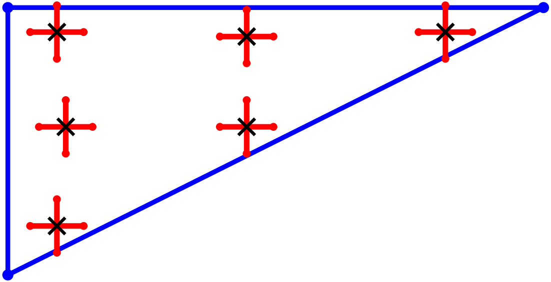


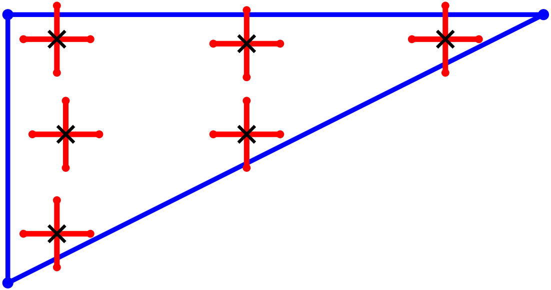


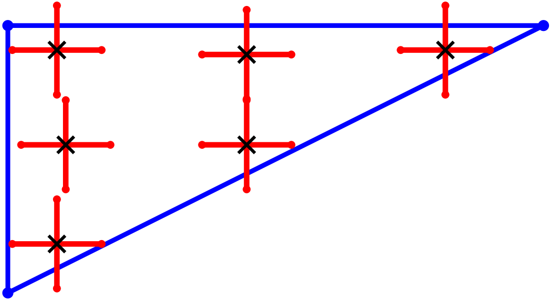


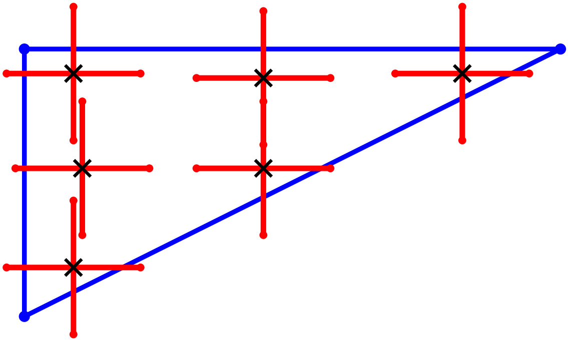


Quasi-continuum method
Mid-beam summation rule (local)

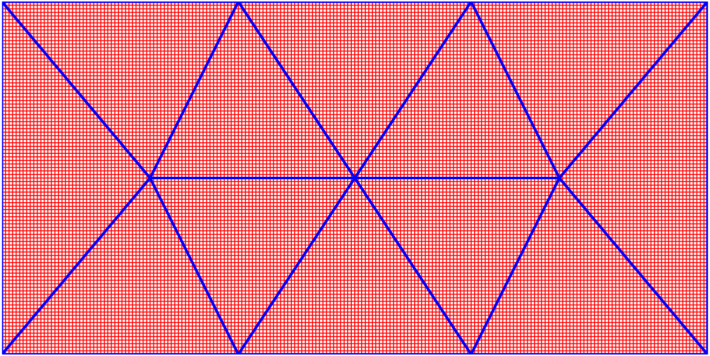






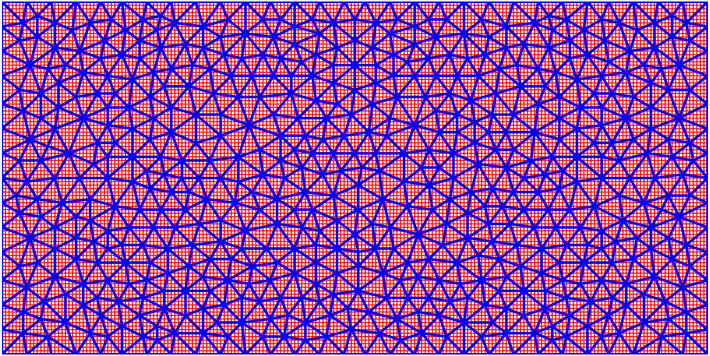


Results
Mesh 1, 12 triangles on $[0, 200] \times [0, 100]$



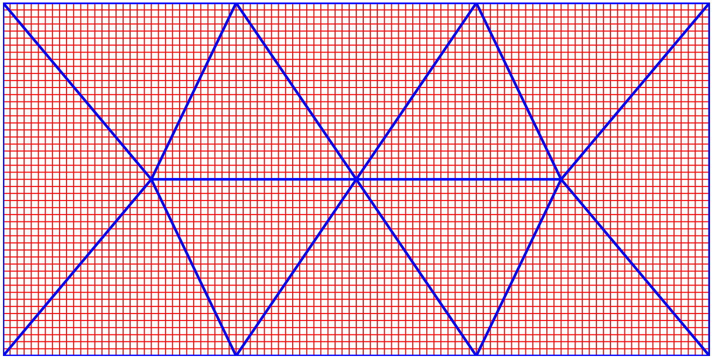
Results

Mesh 12, 1134 triangles on $[0,\ 200] \times [0,\ 100]$



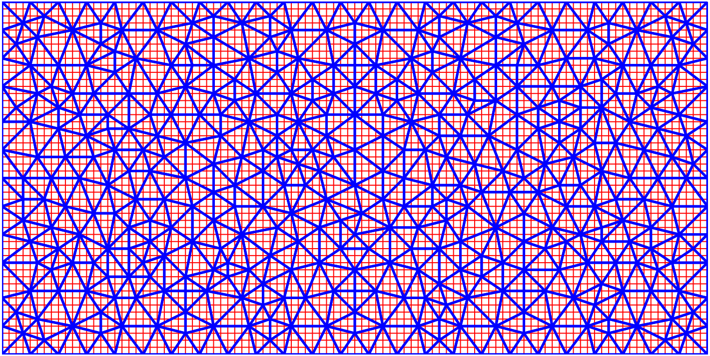
Results

Mesh 1, 12 triangles on $[0, 100] \times [0, 50]$



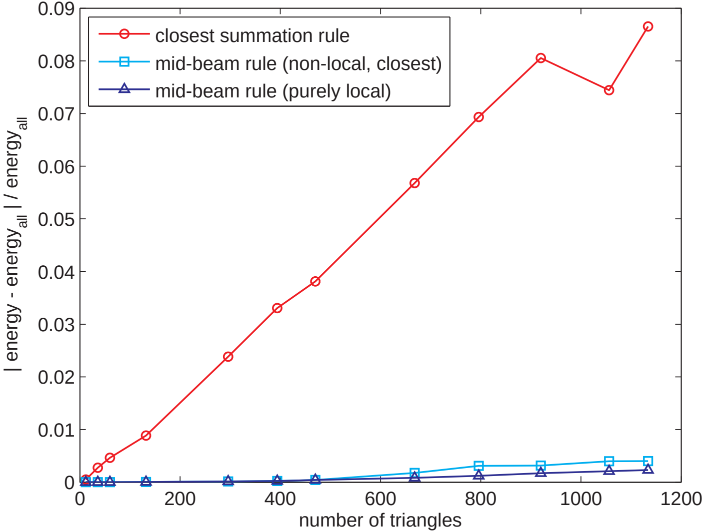
Results

Mesh 9, 796 triangles on $[0,\ 100] \times [0,\ 50]$



Results

Uniaxial test $[0, 200] \times [0, 100]$



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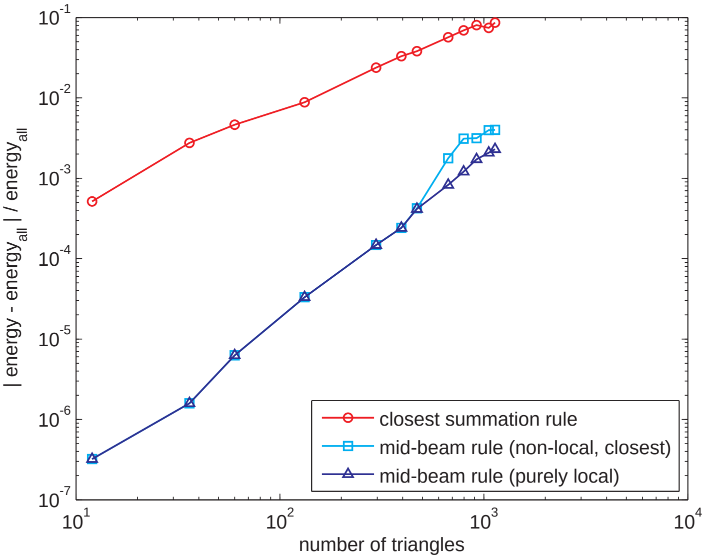
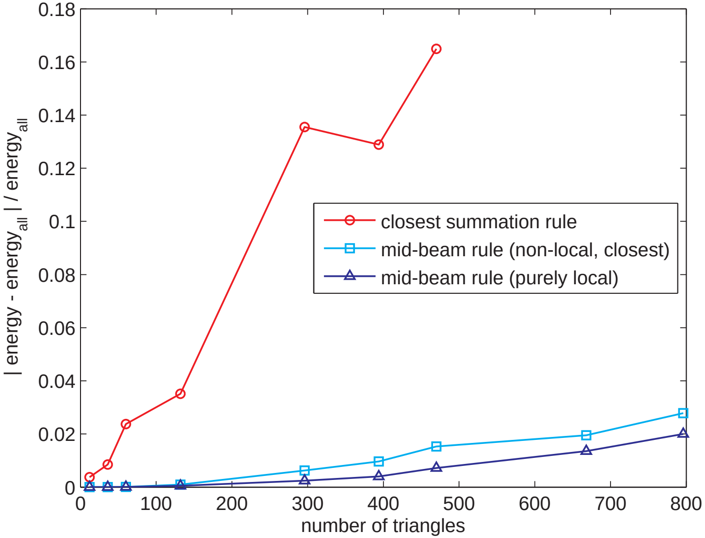
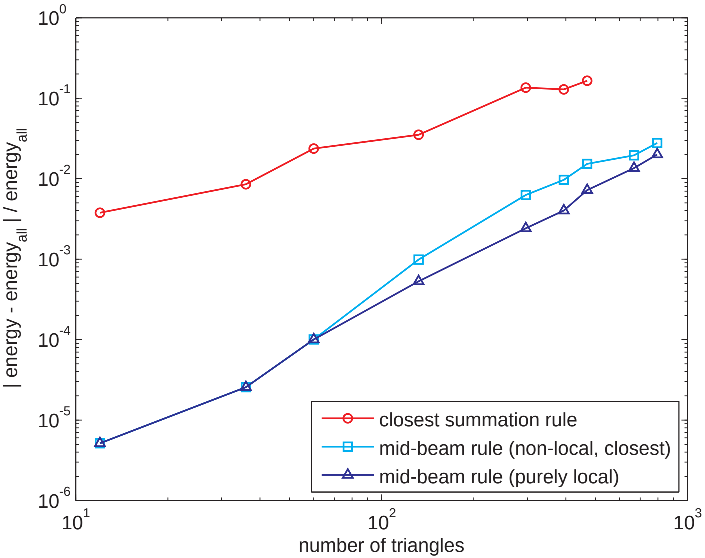



0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
0
100
200
300
400
500
600
700
800
number of triangles
| energy - energy_all | / energy_all
closest summation rule
mid-beam rule (non-local, closest)
mid-beam rule (purely local)

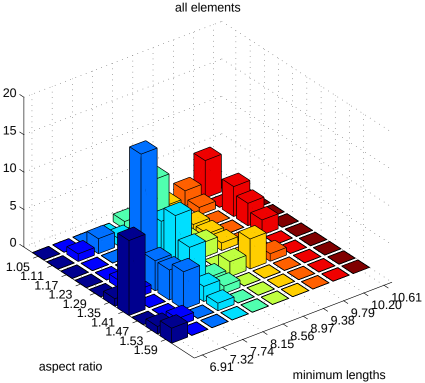
Results

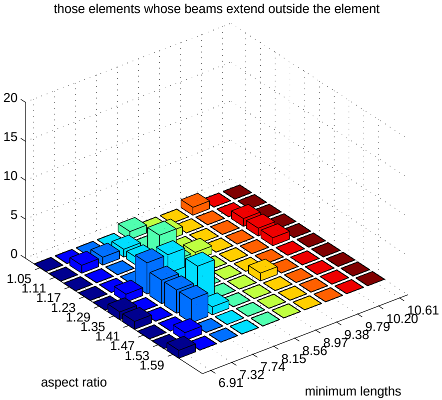
Uniaxial test $[0,\ 100] \times [0,\ 50]$



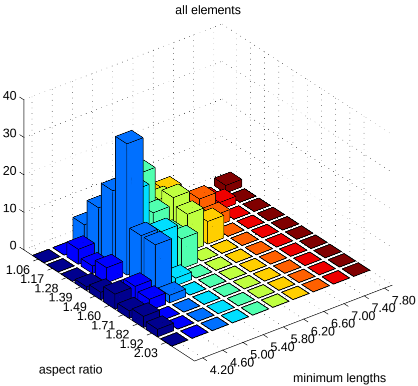
Results

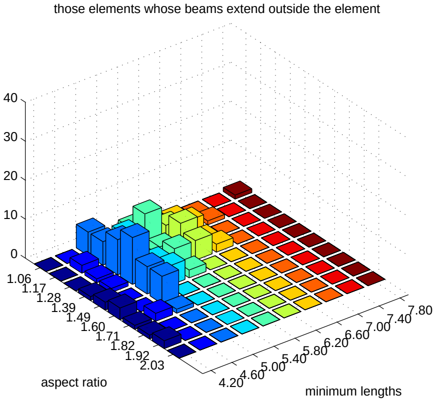
Mesh quality, mesh 4 on $[0, 100] \times [0, 50]$ (**closest beam rule**)





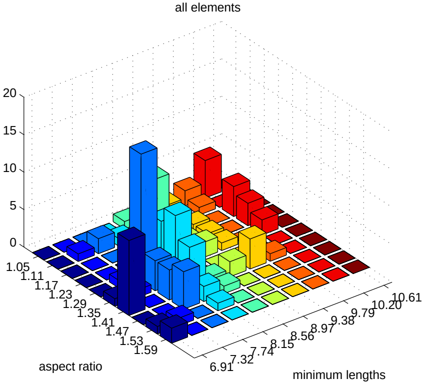
Mesh quality, mesh 5 on $[0, 100] \times [0, 50]$ (**closest beam rule**)

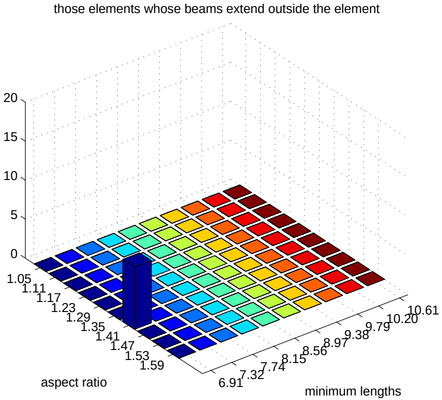




Results

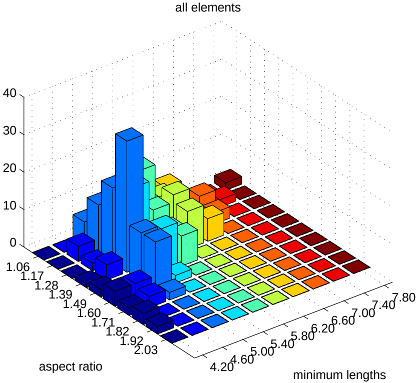
Mesh quality, mesh 4 on $[0, 100] \times [0, 50]$ (mid-beam rule, local)

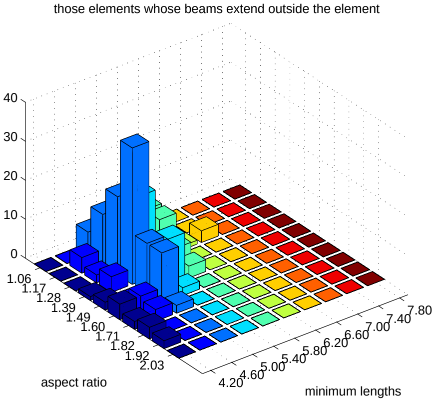




Results

Mesh quality, mesh 5 on $[0, 100] \times [0, 50]$ (**mid-beam rule, local**)





Conclusions and further work

The results show that

- the mid-beam rules have a significantly lower error than the closest summation rule
- of the two mid-beam rules, the local rule performs better than the non-local rule

Current work involves

- running problems with a defect modelled by a fully resolved region

Acknowledgements

EPSRC EP/J01947X/1

Towards rationalised computational expense for simulating fracture over multiple scales.

Dr Pierre Kerfriden.

The internal energy of beam i given in a local coordinate system

$$
\begin{aligned}
E_i &= \frac{\mathcal{E}}{2} \int_V \left(\varepsilon_{xx/u} + \varepsilon_{xx/by} + \varepsilon_{xx/bz}\right)^2 + \frac{\gamma_{xy}^2 + \gamma_{xz}^2}{2(1+\nu)} \, dV \\
&= \frac{\mathcal{E}}{2} \int_V \left(\frac{u_b - u_a}{L} - yv'' - zw''\right)^2 + \left(\frac{\theta_b^x - \theta_a^x}{L}\right)^2 \frac{y^2 + z^2}{2(1+\nu)} \, dV \, .
\end{aligned}
$$

We expand $v(x)$ and $w(x)$ as third degree polynomials and calculate their coefficients by using the following conditions

$$
\begin{aligned}
v(x=0) &= v_a & \qquad w(x=0) &= w_a \\
v(x=L) &= v_b & \qquad w(x=L) &= w_b \\
v'(x=0) &= \theta_a^z & \qquad w'(x=0) &= -\theta_a^y \\
v'(x=L) &= \theta_b^z & \qquad w'(x=L) &= -\theta_b^y \, .
\end{aligned}
$$

Number of triangles out of which sampling beams stray, for the domain $[0, 200] \times [0, 100]$.

mesh #	number of triangles	closest rule	mid-beam rule (non-local)	mid-beam) rule (local)
1	12	0	0	0
2	36	0	0	0
3	60	0	0	0
4	132	0	0	0
5	296	40	0	0
6	394	104	0	0
7	470	163	12	12
8	668	269	89	85
9	796	348	198	198
10	920	393	356	350
11	1056	454	583	571
12	1134	508	738	728

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Number of sampling beams for the domain $[0, 200] \times [0, 100]$. Total number of beams in the lattice: 40300.

mesh #	number of triangles	closest rule		mid-beam rules	
1	12	144	(0.36%)	144	
2	36	432	(1.07%)	432	
3	60	720	(1.79%)	720	
4	132	1584	(3.93%)	1584	
5	296	3552	(8.81%)	3552	
6	394	4726	(11.73%)	4728	(11.73%)
7	470	5631	(13.97%)	5640	(14.00%)
8	668	7936	(19.69%)	8016	(23.70%)
9	796	9359	(23.22%)	9552	(27.39%)
10	920	10685	(26.51%)	11040	(27.39%)
11	1056	12141	(30.13%)	12672	(31.44%)
12	1134	12929	(32.08%)	13608	(33.77%)

Total degrees of freedom of the lattice for the domain $[0, 200] \times [0, 100]$: 121806.

mesh #	number of triangles	degrees of freedom
1	12	300
2	36	813
3	60	1326
4	132	2805
5	296	6108
6	394	8064
7	470	9591
8	668	13542
9	796	16083
10	920	18531
11	1056	21228
12	1134	22764