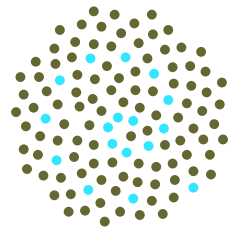


Back to the Surface: Surface magnetisation of the 3-state Potts model

Ian G. Enting

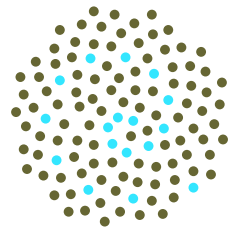
Centre of Excellence for Mathematics and Statistics of Complex Systems
(MASCOS)

Acknowledgements



- ▶ Tony Guttman — 25 years of collaboration
- ▶ Lattice statistics group at University of Melbourne
- ▶ Tom de Neef — who introduced me to Finite Lattice Method.
- ▶ My fellowship at MASCOS is supported by CSIRO sponsorship
- ▶ The Centre of Excellence in Mathematics and Statistics of Complex Systems (MASCOS) is funded by the ARC

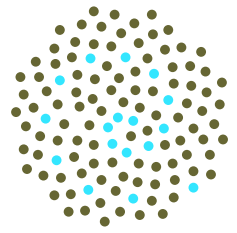
Why bother*



- ▶ Because we can
- ▶ Revisit/commemorate my first Guttman collaboration — Ising surface χ — and 25 subsequent papers
- ▶ Applications, especially surface percolation
- ▶ Reference case for Monte Carlo techniques used in applications
- ▶ Develop code for using variational boundary conditions to extend bulk series

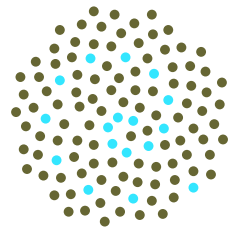
*A term also applied to cappacini made from soy milk and decaffeinated coffee.

What surface series?

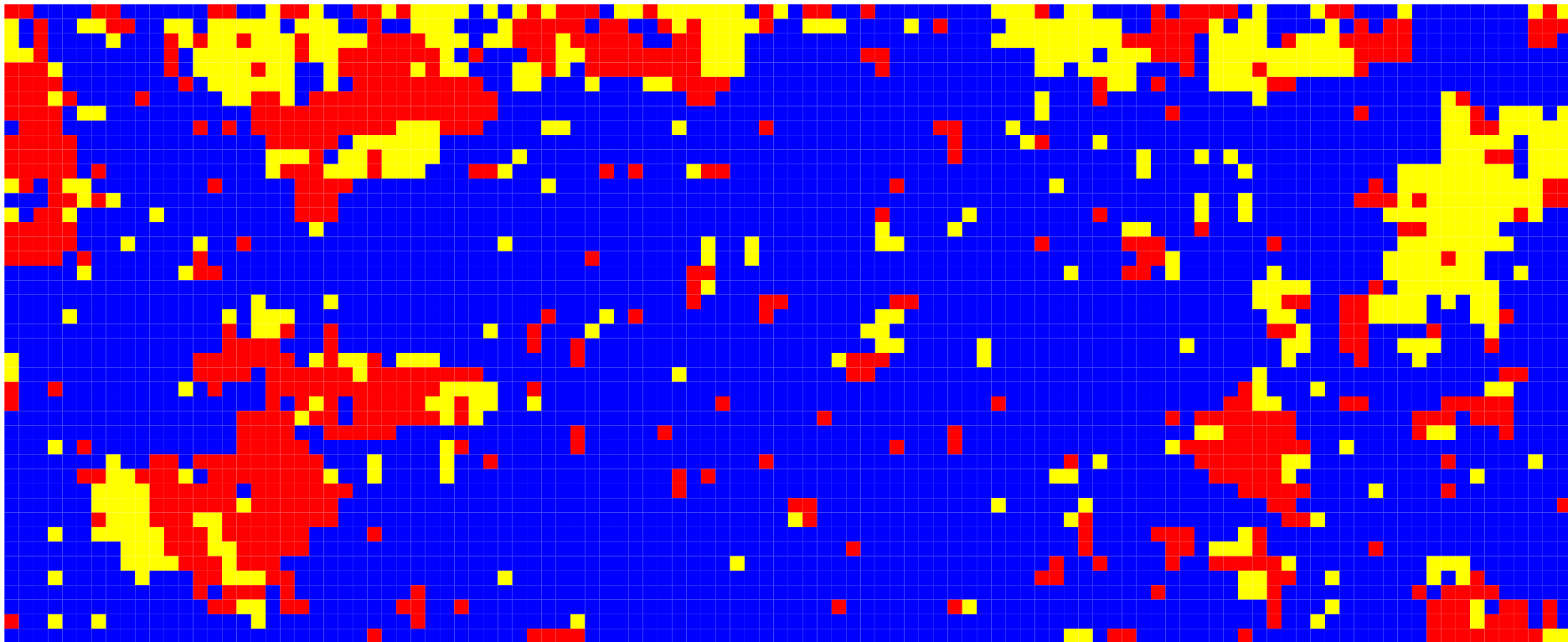


- ▶ Free or fixed boundaries — have done both
- ▶ Free energy of $N \times N$ square lattice
$$F(T, H, H_1) = N^2 f(T, H) + 4N f_s(T, H, H_1)$$
- ▶ Surface corrections from $f_s(T, H, H_1 = 0)$ — exponents related to bulk exponents, e.g.
$$\beta_s = \beta - \nu$$
- ▶ Derivatives with respect to H_1 introduce an independent scaling exponent — for Potts model, this is known from conformal invariance (Cardy, 1984).

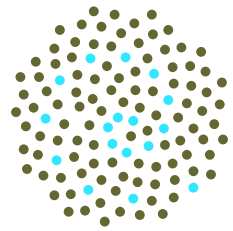
Monte Carlo



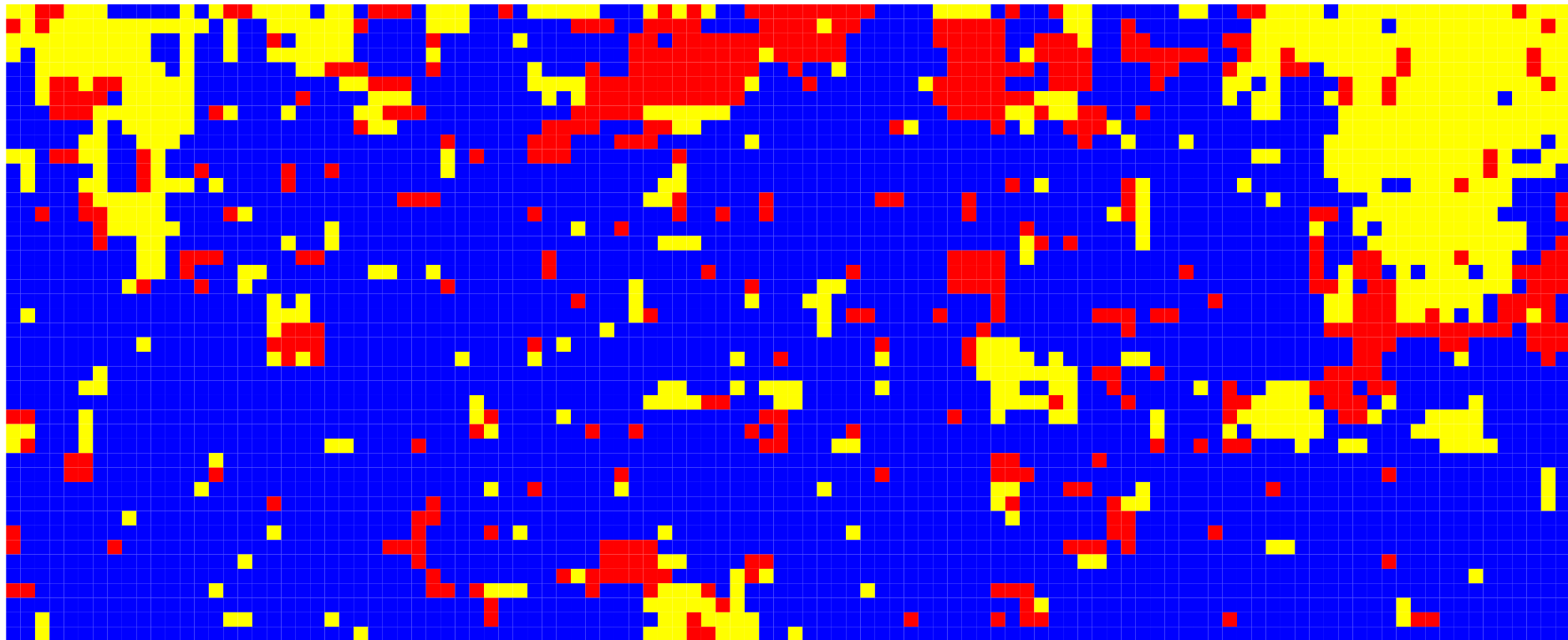
Free upper boundary $z = 0.362$ ($z_c = 0.36607..$)



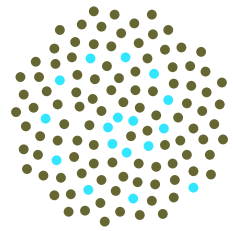
Monte Carlo



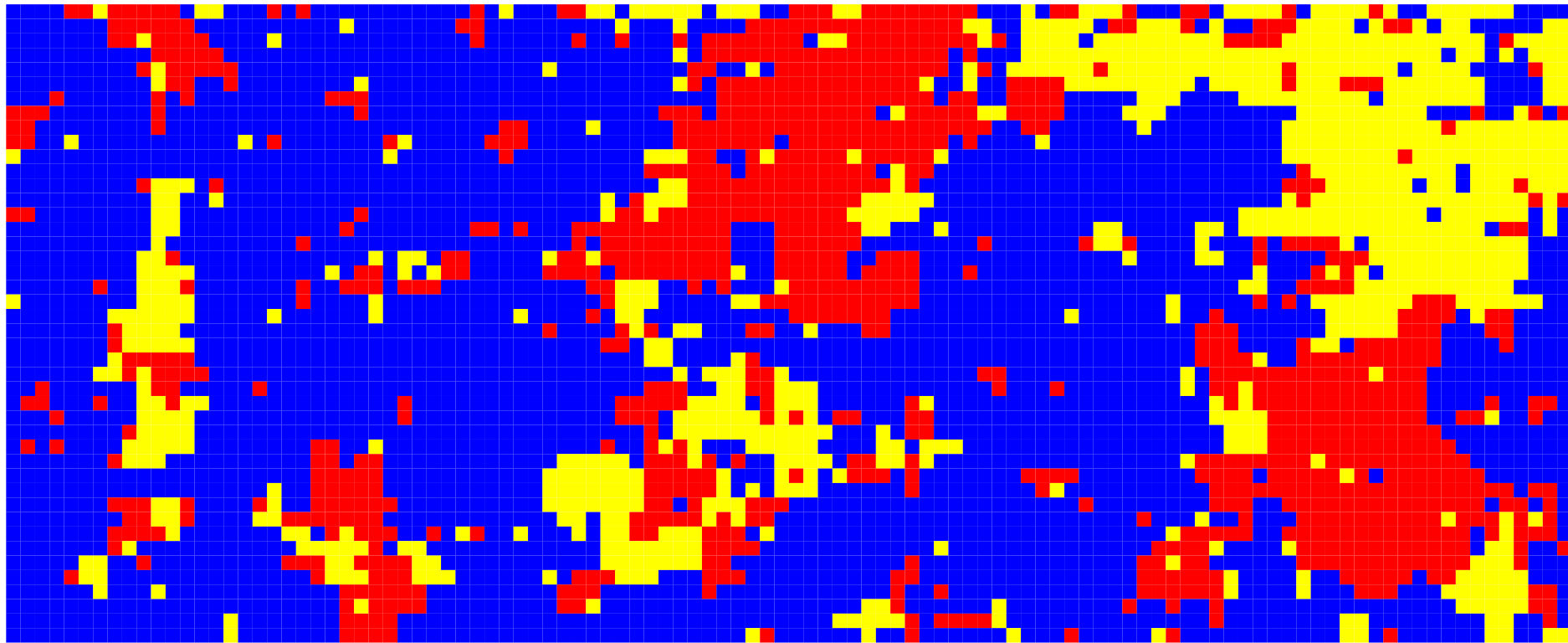
Free upper boundary $z = 0.362$ ($z_c = 0.36607..$)



Monte Carlo

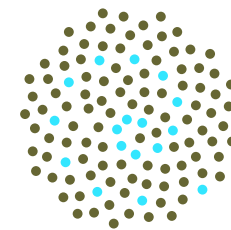


Free upper boundary $z = 0.362$ ($z_c = 0.36607..$)



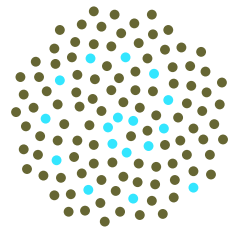
Occasional large fluctuations.

Thermodynamic fns



- ▶ Take fully aligned state as zero of energy
- ▶ Corresponding partition function is Λ
- ▶ Expand in $z = \exp(-J/k_B T)$
and $x = 1 - \exp(-H/k_B T)$ and
 $x_1 = 1 - \exp(-H_1/k_B T)$ to order x^1 and x_1^1
- ▶ Working with $\Lambda_s^2 = \exp(2f_s)$ requires only integers
- ▶ M_1 and M_s from appropriate derivatives.

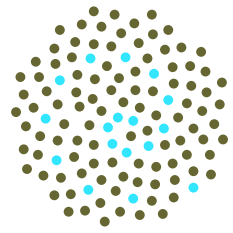
Finite Lattice Method (FLM)



The two components of the FLM are:

- ▶ combinatorics — which linear combinations of finite (rectangular) lattice free energies?
- ▶ computation — calculating the free energies:
 - ▶ transfer matrix: build up rectangle column by column
 - ▶ ** sparse matrix factorisation of transfer matrix: build up rectangle one site at a time
 - ▶ pivoting: fix a ‘radial’ section and pivot around centre (Enting, Guttmann and Jensen)

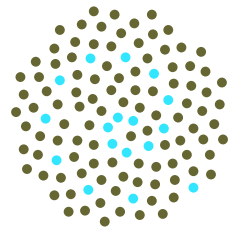
Combinatorics



- ▶ $f(T, H) \approx \sum_{mn} a_{mn} f_{mn}(T, H)$
- ▶ $f_s(T, H, H_1 = 0) \approx \sum_{mn} d_{mn} f_{mn}$ if b.c. match form of expansion — low- T fixed , high- T free
- ▶ $f_s(T, H, H_1) \approx \sum_{mn} [b_{mn} g_{mn}(T, H, H_1) + c_{mn} f_{mn}(T, H)]$
 - ▶ Bulk = cancel surface, $\sum_{nm} n \times a_{mn} = 0$
 - ▶ Surface = cancel bulk $\sum_{nm} nm \times d_{mn} = 0$
- ▶ a_{mn} etc. from inverses of truncated incidence matrices.
- ▶ Exponentiate all this: $\prod [\text{partition functions}]^{a_{mn}}$, etc.

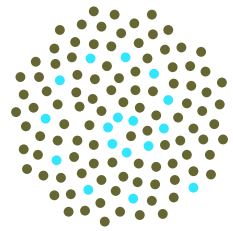
To make a statue of an elephant, take a piece of stone and cut off whatever doesn't look like an elephant

Transfer Matrix Calculations



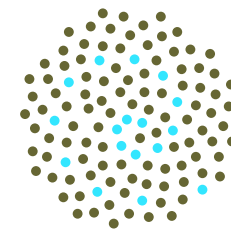
- ▶ For width w , vector has q^w elements.
- ▶ Never actually store the ‘transfer matrix’, determine elements from indices.
- ▶ Adding one site at a time represents a sparse-matrix factorisation of row-by-row approach
 - complexity goes from $(q^w)^2$ to $qw \times q^w$
- ▶ Three cases: (i) bulk case (fixed b.c. always); (ii) boundary before first column; (iii) boundary along lower edge.

The series: Free b.c.



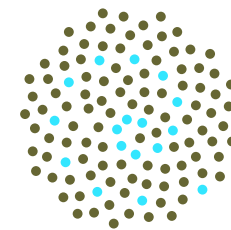
n	Λ_s^2	M_1	M_s	n	Λ_s^2	M_1	M_s
0	1	1	0	13	5368	-7668	-40341
1	0	0	0	14	8682	-19380	-101151
2	0	0	0	15	24710	-44388	-280860
3	4	-3	-3	16	64226	-112725	-759630
4	0	-6	-3	17	123238	-263523	-1979973
5	12	-18	-21	18	383920	-673302	-5542941
6	14	-33	-33	19	819806	-1633077	-14537274
7	22	-69	-108	20	2065562	-4158477	-39688650
8	106	-141	-297	21	5542422	-10382247	-107430594
9	80	-264	-672	22	12354142	-26395017	-287271708
10	432	-648	-2124	23	33865704	-66703539	-783774780
11	818	-1332	-5340	24	82302072	-170292129	-2107671147
12	1460	-3420	-14043	25	203861976	-432697869	-5695479651

The series: Fixed b.c.



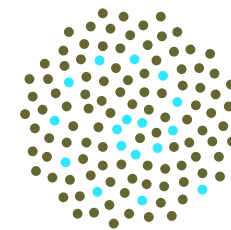
n	Λ_s^2	M_1	M_s	n	Λ_s^2	M_1	M_s
0	1	1	0	11	-130	-153	450
1	0	0	0	12	-388	-504	1923
2	0	0	0	13	-620	-330	3369
3	0	0	0	14	-2394	-2415	14841
4	0	-3	0	15	-4370	-3558	29919
5	0	0	0	16	-12118	-7029	102192
6	-2	-9	3	17	-32314	-28341	258912
7	-2	-9	3	18	-68356	-32862	733956
8	-10	-12	27	19	-199862	-134628	1999521
9	-24	-60	54	20	-466754	-281472	5630457
10	-52	-48	216	21	-1160486	-564627	14781231

The series: Fixed b.c.



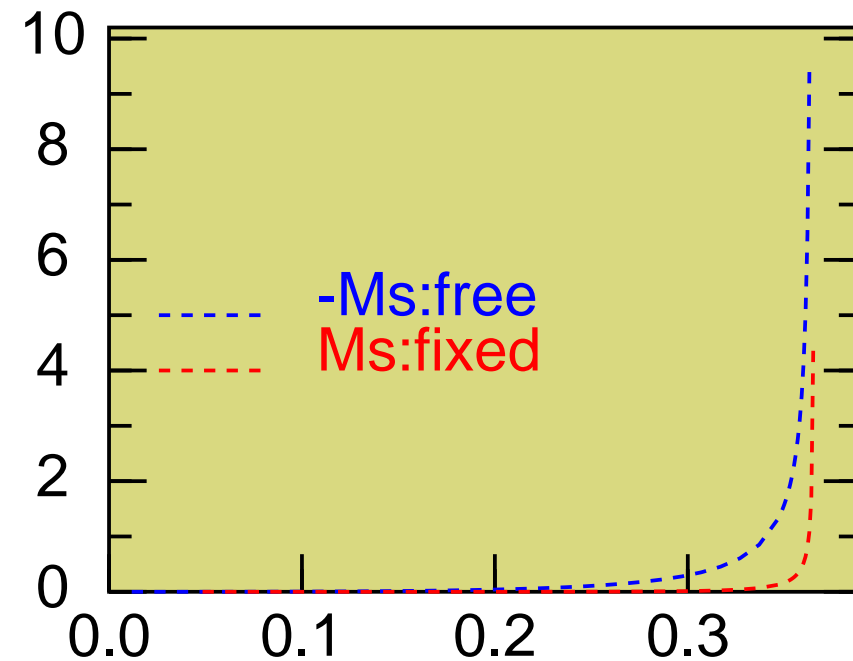
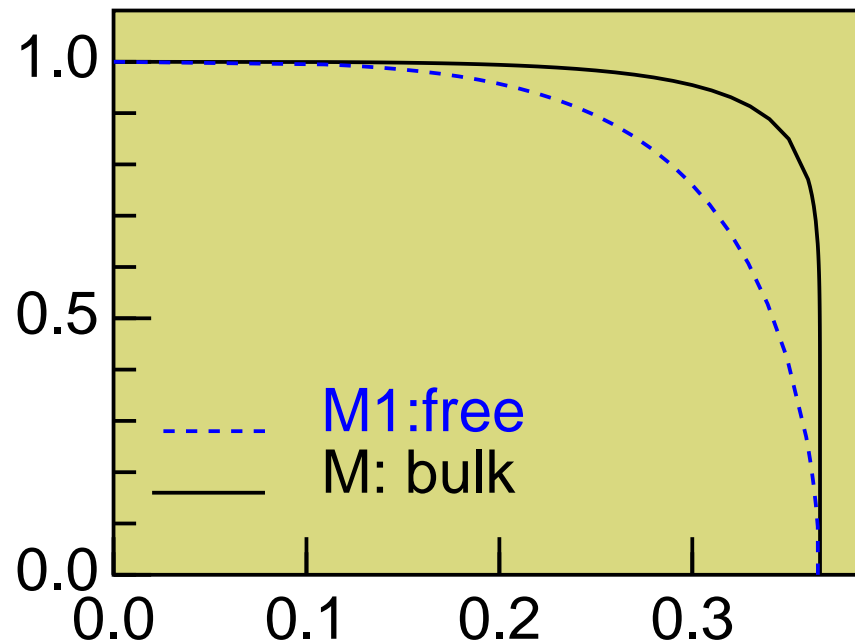
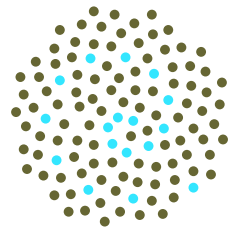
n	Λ_s^2	M_1	M_s
22	-3157190	-1875285	42871278
23	-7370600	-3433521	111503781
24	-19832164	-9703338	316807263
25	-50098568	-24527004	851747649
26	-124733230	-52280256	2334828861
27	-333519798	-152141355	6414892248
28	-827189010	-340328889	17438442444
29	-2163220720	-865856643	47668778127
30	-5605295194	-2270118705	130703758041
31	-14236383324	-5261117598	354352750362
32	-37525063234	-14115364374	973753722000
33	-96153861050	-34571651562	2645183086965
34	-250010407376	-86429776635	7228699923906

The series: Fixed b.c.



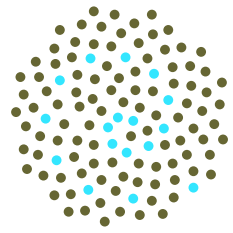
n	Λ_s^2	M_1	M_s
35	-653687531246	-225963265485	19732827586044
36	-1686617537120	-553507149000	53736713238600
37	-4426354756414	-1437344123532	146761454268627
38	-11515945714078	-3648952254324	400043201310129
39	-30043995520112	-9202758880908	1090373595142140
40	-78842242959410	-23907568780911	2975993658025665
41	-205627206729564	-60390785024094	8106170375325594
42	-539962216165134	-155620455564495	22114015704445812
43	-1415813195688816	-400541562312582	60279224508672003
44	-3712050559013522	-1022685297476403	164296584793395933
45	-9769216758495434	-2651300383803702	448027804527081864
46	-25653952409425890	-6806590215847512	1220988919790522244
47	-67542769159197940	-17573483170034106	3328616271906352083

Plots



Scaling predicts M_s has exponent $\beta_s = -13/18$
Conformal invariance predicts $\beta_1 = 5/9$ for M_1
Bulk magnetisation has exponent $\beta = 1/9$

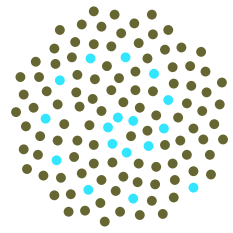
Analysis of series



Mainly using 2nd-order differential approximants.

- ▶ Ratios not usable, dlog Padés mostly scattered
- ▶ Series for free boundaries are quite short:
Padés to dlog M_1 give $\beta_1 = 0.50 \pm 0.5$
Padés and DAs for M_s have wide scatter for β_s
- ▶ With fixed boundaries:
 M_s close to scaling, but systematic difference
 $M_1(z_c) \neq 0$, biased DA estimates: $\beta_1 = 0.65 \pm 0.05$
- ▶ No indication of confluent singularities
(but if $\Delta \approx 0.5$, then $\beta_1 + \Delta \approx \text{integer}$).

Future directions



- ▶ More efficient counting for free boundaries
- ▶ Susceptibilities: fluctuations
- ▶ High temperature series
- ▶ Percolation as $q \rightarrow 1$ limit
- ▶ Bounds on $M_{1:\text{fixed}}$
- ▶ Apply boundary field(s) as variational variable(s) — does this lead to longer bulk series?