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

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(MASCOS)

Acknowledgements

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Why bother*

- Because we can
- Revisit/commemorate my first Guttmann 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

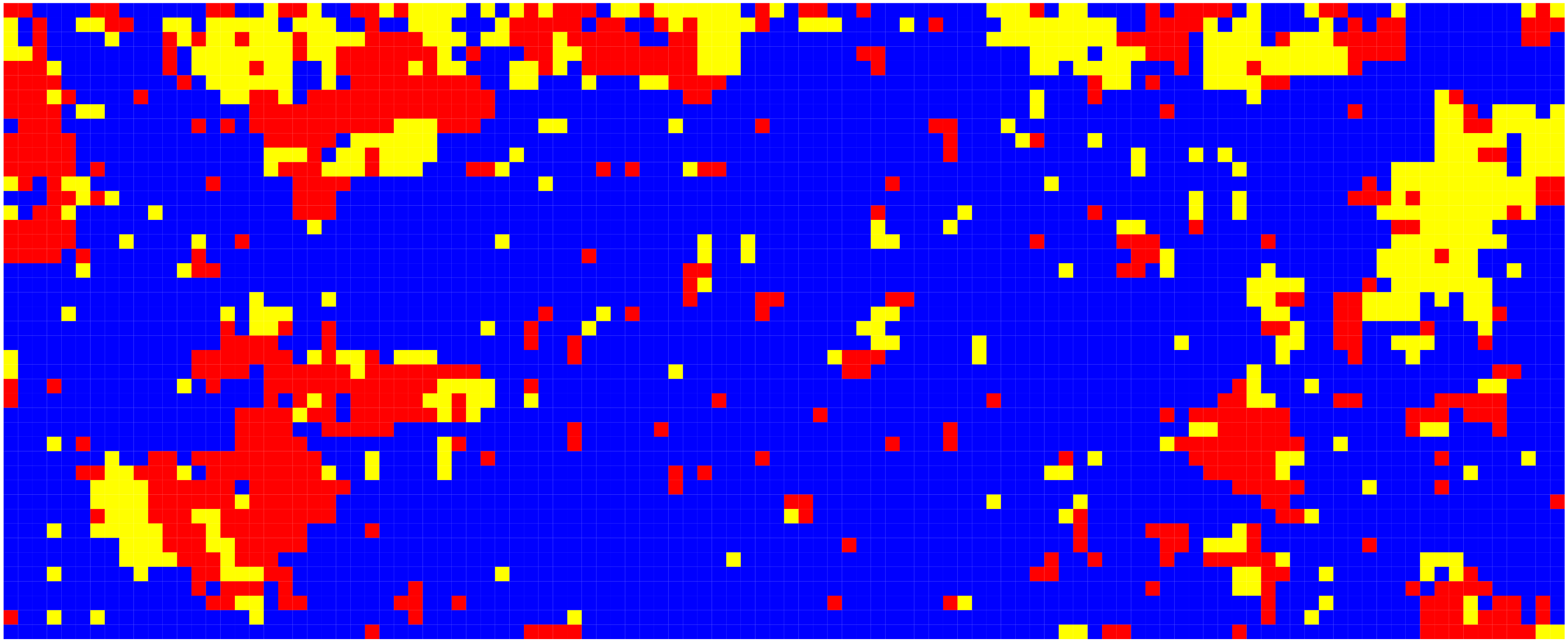
*A term also applied to cappacini made from soy milk and decaffeinated coffee.

What surface series?

- Free or fixed boundaries — have done both
- Free energy of $N \times N$ square lattice
  $F(T, H, H_1) = N^2 f(T, H) + 4N f_\mathrm{s}(T, H, H_1)$
- Surface corrections from $f_\mathrm{s}(T, H, H_1 = 0)$ — exponents related to bulk exponents, e.g. $\beta_\mathrm{s} = \beta - \nu$
- 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 $z = 0.362$ ($z_c = 0.36607..$)



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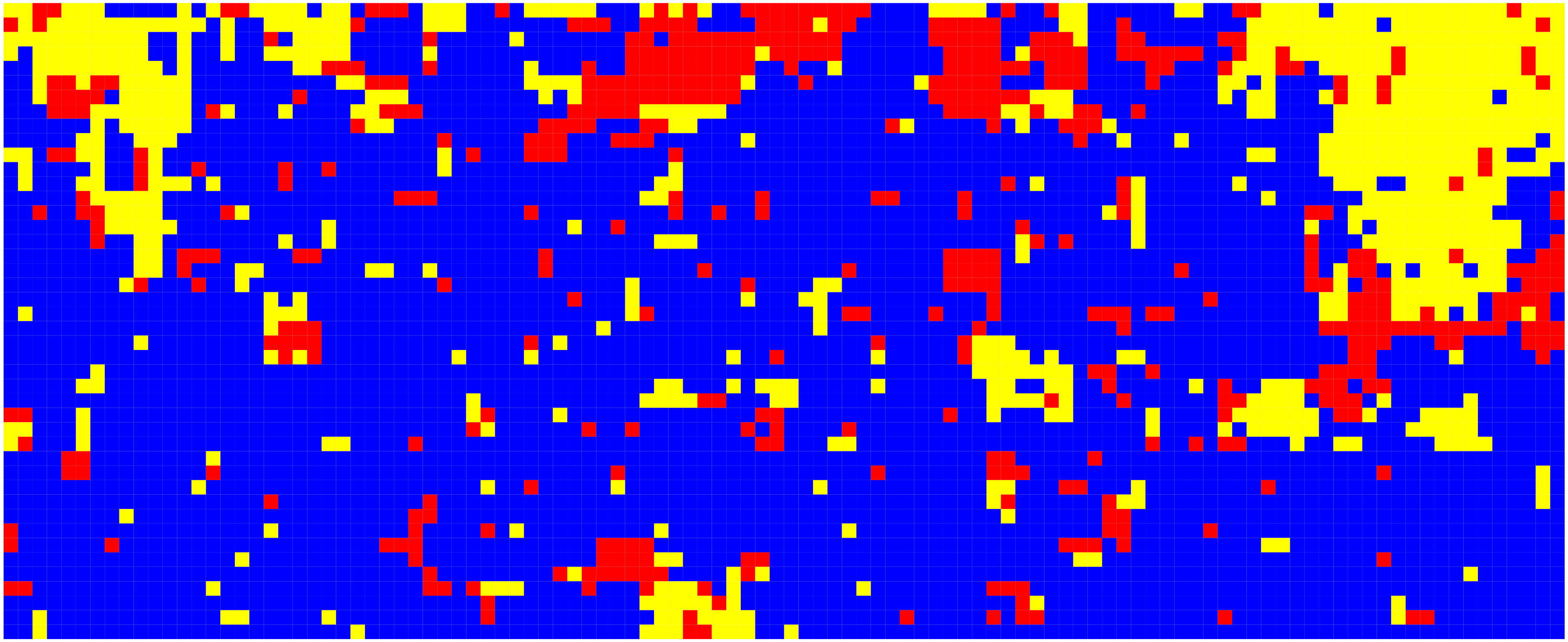

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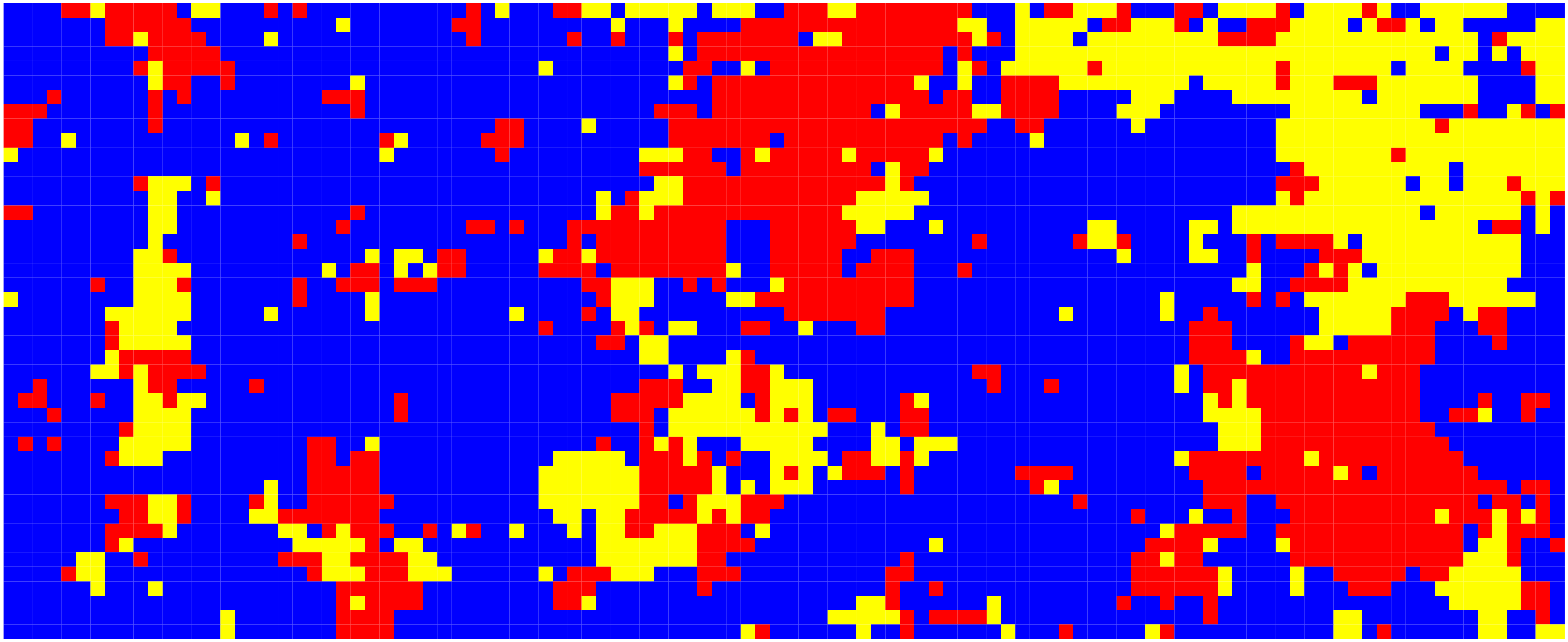


Occasional large fluctuations.

Thermodynamic fns

- Take fully alligned state as zero of energy
- Corresponding partition function is Λ
- Expand in $z = \exp(-J/k_{\mathrm{B}}T)$ and $x = 1 - \exp(-H/k_{\mathrm{B}}T)$ and $x_1 = 1 - \exp(-H_1/k_{\mathrm{B}}T)$ to order x^1 and x_1^1
- Working with $\Lambda_{\mathrm{s}}^2 = \exp(2f_{\mathrm{s}})$ 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: $\prod$ [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
0	1	1	0
1	0	0	0
2	0	0	0
3	4	−3	−3
4	0	−6	−3
5	12	−18	−21
6	14	−33	−33
7	22	−69	−108
8	106	−141	−297
9	80	−264	−672
10	432	−648	−2124
11	818	−1332	−5340
12	1460	−3420	−14043

n	Λ_s^2	M_1	M_s
13	5368	−7668	−40341
14	8682	−19380	−101151
15	24710	−44388	−280860
16	64226	−112725	−759630
17	123238	−263523	−1979973
18	383920	−673302	−5542941
19	819806	−1633077	−14537274
20	2065562	−4158477	−39688650
21	5542422	−10382247	−107430594
22	12354142	−26395017	−287271708
23	33865704	−66703539	−783774780
24	82302072	−170292129	−2107671147
25	203861976	−432697869	−5695479651

The series: Fixed b.c.

n	Λ_s^2	M_1	M_s
0	1	1	0
1	0	0	0
2	0	0	0
3	0	0	0
4	0	−3	0
5	0	0	0
6	−2	−9	3
7	−2	−9	3
8	−10	−12	27
9	−24	−60	54
10	−52	−48	216

n	Λ_s^2	M_1	M_s
11	−130	−153	450
12	−388	−504	1923
13	−620	−330	3369
14	−2394	−2415	14841
15	−4370	−3558	29919
16	−12118	−7029	102192
17	−32314	−28341	258912
18	−68356	−32862	733956
19	−199862	−134628	1999521
20	−466754	−281472	5630457
21	−1160486	−564627	14781231

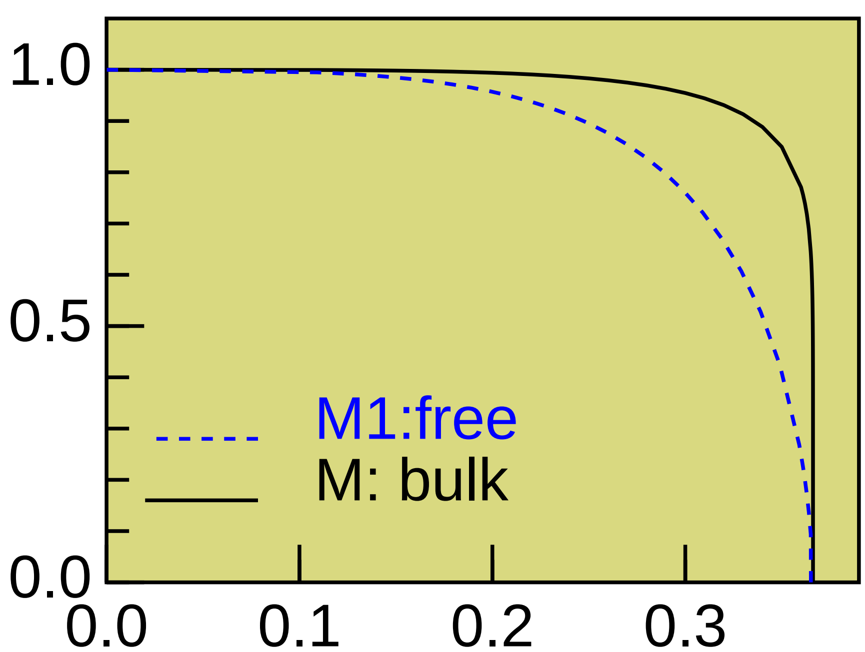
The series: Fixed b.c.

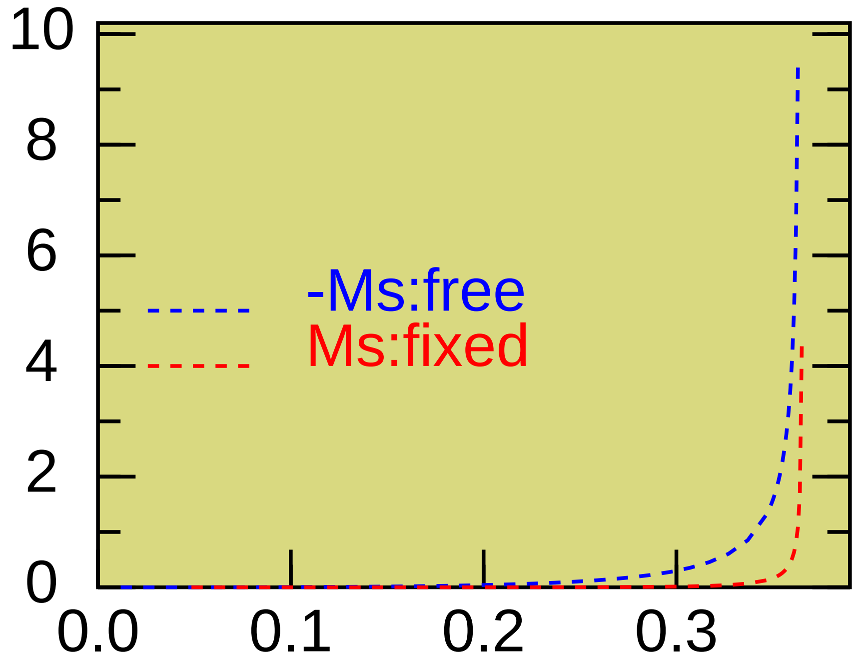
n	Λ_s^2	M_1	M_s
22	-3157190	-1875285	42871278
23	-7370600	-3433521	111503781
24	-19832164	-9703338	316807263
25	-50098568	-24527004	851747649
26	-124733230	-52280256	2334828861
27	-333519798	-152141355	6414892248
28	-827189010	-340328889	17438442444
29	-2163220720	-865856643	47668778127
30	-5605295194	-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 $M_{\rm s}$ has exponent $\beta_{\rm s} = -13/18$

Conformal invariance predicts $\beta_1 = 5/9$ for M_1

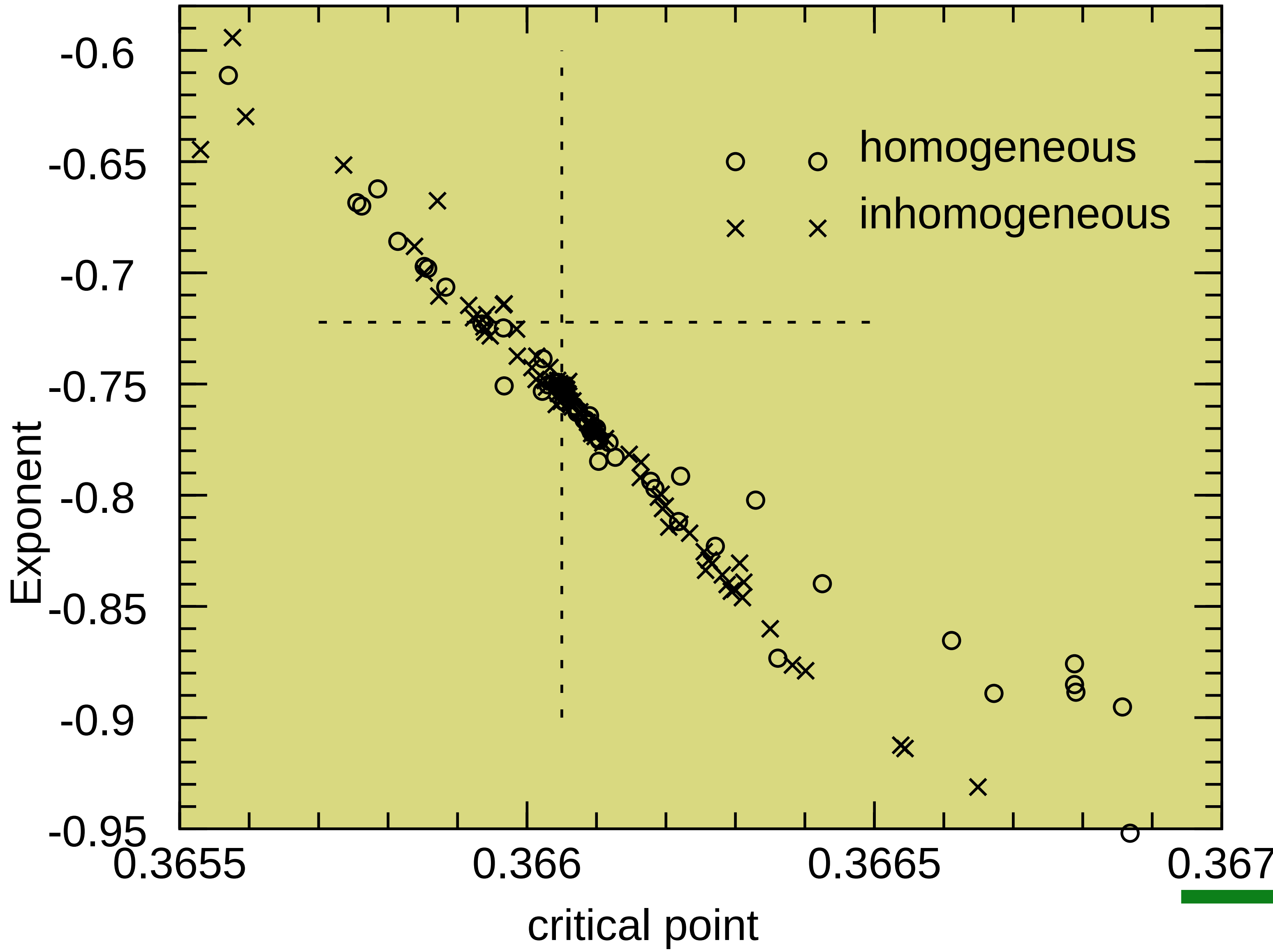
Bulk magnetisation has exponent $\beta = 1/9$

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
  $M_1(z_\mathrm{c}) \neq 0$, biased DA estimates: $\beta_1 = 0.65 \pm 0.05$
- No indication of confluent singularities
  (but if $\Delta \approx 0.5$, then $\beta_1 + \Delta \approx$ integer).

Fixed b.c.: DAs for M_S



Future directions

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