

Supporting Information

Algorithms for Fitting Generalized Power Diagrams to 3D Image Data: A Prerequisite for Virtual Materials Testing

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July 7, 2026

S1 Quantitative performance evaluation

	Voronoi	Laguerre			d-GBPD		GBPD			
	GD	Hq	Neper	CE	GD	GD	GD	LP	H ₀	Hq
AlCuStep0	0.104	0.069	0.015	0.036	0.067	0.032	0.017	0.068	0.012	0.011
AlCuStep20	0.093	0.065	0.017	0.033	0.062	0.024	0.015	0.013	0.012	0.011
AlCuStep60	0.094	0.071	0.021	0.039	0.071	0.023	0.014	0.048	0.012	0.011
PureFeStep0	0.153	0.128	0.082	0.149	0.115	0.051	0.025	0.059	0.029	0.022
Ceramic	0.016	0.046	0.008	0.010	0.010	0.014	0.030	0.014	0.014	0.009
WIND	0.053	0.079	0.014	0.040	0.025	0.020	0.024	0.016	0.016	0.012
Zinc1	0.141	0.127	0.044	0.101	0.098	0.055	0.025	0.037	0.025	0.019
Zinc2	0.113	0.090	0.037	0.071	0.081	0.046	0.029	0.041	0.021	0.016

Table S1: Values of F_{φ_d} achieved by deploying the considered fitting methods to the different data sets.

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	Voronoi	Laguerre			d-GBPD		GBPD			
	GD	Hq	Neper	CE	GD	GD	GD	LP	H ₀	Hq
AlCuStep0	0.238	0.122	0.065	0.074	0.171	0.066	0.042	0.142	0.034	0.040
AlCuStep20	0.215	0.115	0.066	0.068	0.158	0.057	0.037	0.035	0.035	0.039
AlCuStep60	0.234	0.188	0.140	0.138	0.194	0.103	0.107	0.127	0.111	0.111
PureFeStep0	0.347	0.235	0.164	0.239	0.289	0.137	0.066	0.100	0.058	0.053
Ceramic	0.077	0.105	0.073	0.077	0.074	0.076	0.086	0.075	0.077	0.079
WIND	0.095	0.091	0.028	0.048	0.062	0.038	0.053	0.037	0.037	0.039
Zinc1	0.288	0.232	0.128	0.190	0.225	0.115	0.072	0.091	0.111	0.110
Zinc2	0.268	0.196	0.132	0.170	0.212	0.104	0.084	0.100	0.107	0.103

Table S2: Values of F_{φ_A} achieved by deploying the considered fitting methods to the different data sets.

	Voronoi	Laguerre			d-GBPD		GBPD			
	GD	Hq	Neper	CE	GD	GD	GD	LP	H ₀	Hq
AlCuStep0	0.176	0.112	0.106	0.109	0.153	0.072	0.043	0.059	0.029	0.030
AlCuStep20	0.174	0.102	0.106	0.098	0.160	0.057	0.040	0.034	0.030	0.030
AlCuStep60	0.174	0.119	0.118	0.111	0.155	0.056	0.036	0.045	0.033	0.032
PureFeStep0	0.245	0.229	0.230	0.235	0.227	0.131	0.059	0.072	0.068	0.066
Ceramic	0.071	0.165	0.068	0.085	0.073	0.049	0.073	0.037	0.040	0.038
WIND	0.110	0.190	0.092	0.096	0.085	0.056	0.059	0.059	0.063	0.060
Zinc1	0.220	0.207	0.212	0.202	0.209	0.109	0.060	0.054	0.059	0.058
Zinc2	0.198	0.179	0.165	0.177	0.176	0.085	0.068	0.054	0.056	0.055

Table S3: Values of $F_{\varphi_{elo}}$ achieved by deploying the considered fitting methods to the different data sets.

	Voronoi	Laguerre			d-GBPD		GBPD			
	GD	Hq	Neper	CE	GD	GD	GD	LP	H ₀	Hq
AlCuStep0	0.159	0.113	0.087	0.097	0.143	0.071	0.044	0.056	0.031	0.032
AlCuStep20	0.147	0.116	0.094	0.103	0.140	0.060	0.043	0.032	0.029	0.030
AlCuStep60	0.156	0.122	0.099	0.101	0.139	0.058	0.044	0.042	0.030	0.030
PureFeStep0	0.257	0.264	0.227	0.254	0.247	0.159	0.066	0.071	0.068	0.066
Ceramic	0.098	0.137	0.088	0.103	0.098	0.060	0.087	0.048	0.048	0.049
WIND	0.106	0.148	0.096	0.090	0.089	0.068	0.080	0.061	0.062	0.062
Zinc1	0.251	0.249	0.239	0.251	0.247	0.141	0.078	0.059	0.058	0.058
Zinc2	0.189	0.161	0.161	0.177	0.171	0.089	0.076	0.053	0.051	0.051

Table S4: Values of $F_{\varphi_{flat}}$ achieved by deploying the considered fitting methods to the different data sets.

	Voronoi	Laguerre			d-GBPD		GBPD			
	GD	Hq	Neper	CE	GD	GD	GD	LP	H ₀	Hq
AlCuStep0	0.750	0.862	0.903	0.879	0.824	0.854	0.945	0.820	0.945	0.938
AlCuStep20	0.798	0.875	0.911	0.890	0.843	0.874	0.959	0.946	0.948	0.946
AlCuStep60	0.806	0.874	0.913	0.886	0.855	0.871	0.949	0.866	0.939	0.938
PureFeStep0	0.660	0.689	0.714	0.519	0.718	0.754	0.880	0.838	0.879	0.881
Ceramic	0.935	0.882	0.944	0.919	0.936	0.954	0.928	0.950	0.955	0.949
WIND	0.874	0.843	0.910	0.880	0.920	0.928	0.903	0.912	0.916	0.902
Zinc1	0.698	0.733	0.789	0.689	0.761	0.738	0.900	0.865	0.905	0.901
Zinc2	0.722	0.787	0.833	0.757	0.787	0.810	0.903	0.885	0.917	0.912

Table S5: Values of F_{IoU} achieved by deploying the considered fitting methods to the different data sets.

S2 Visual validation

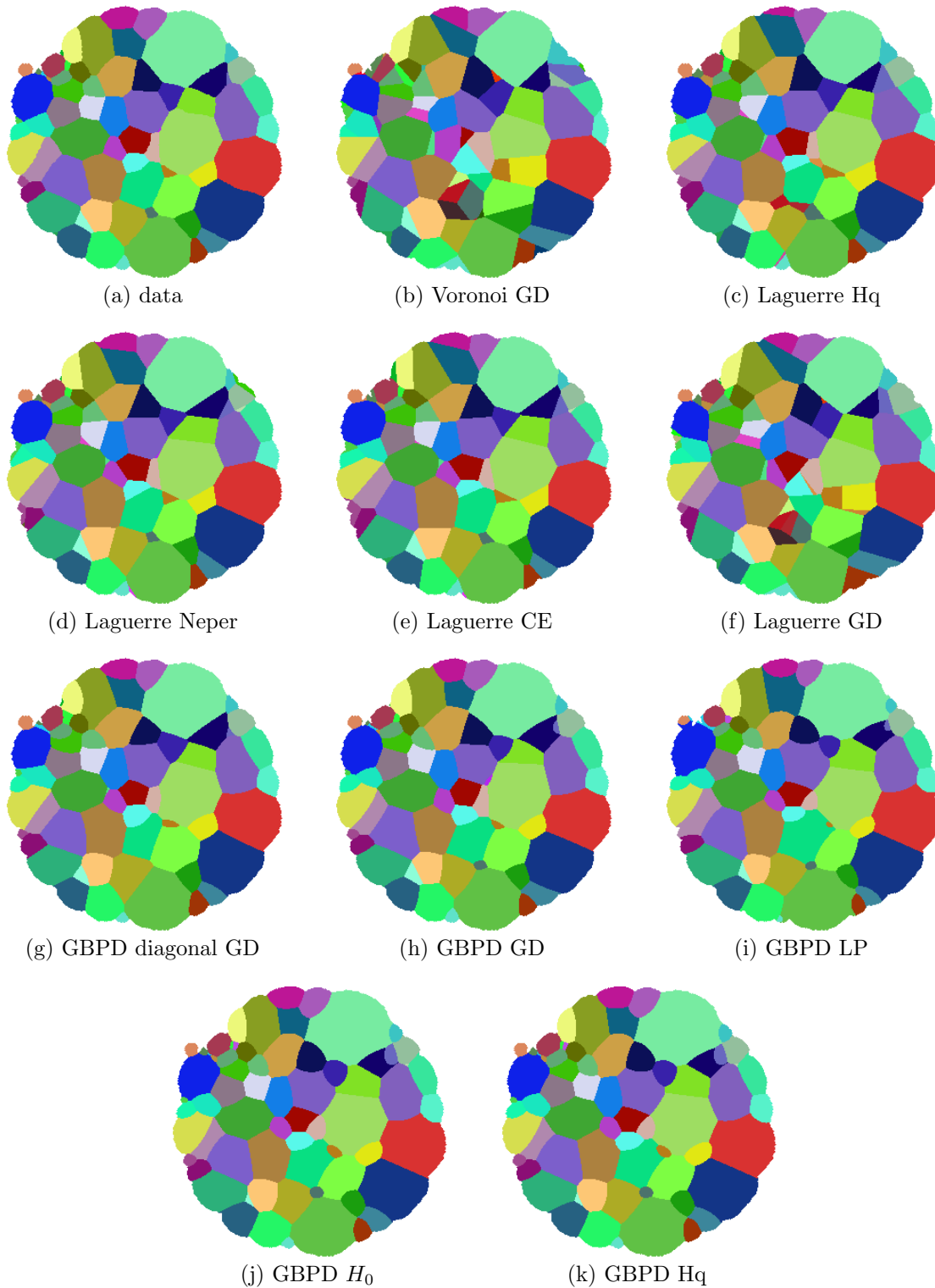


Figure S1: Cross sections of the **AICuStep0** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using Hq (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i), H_0 (j) and Hq (k).

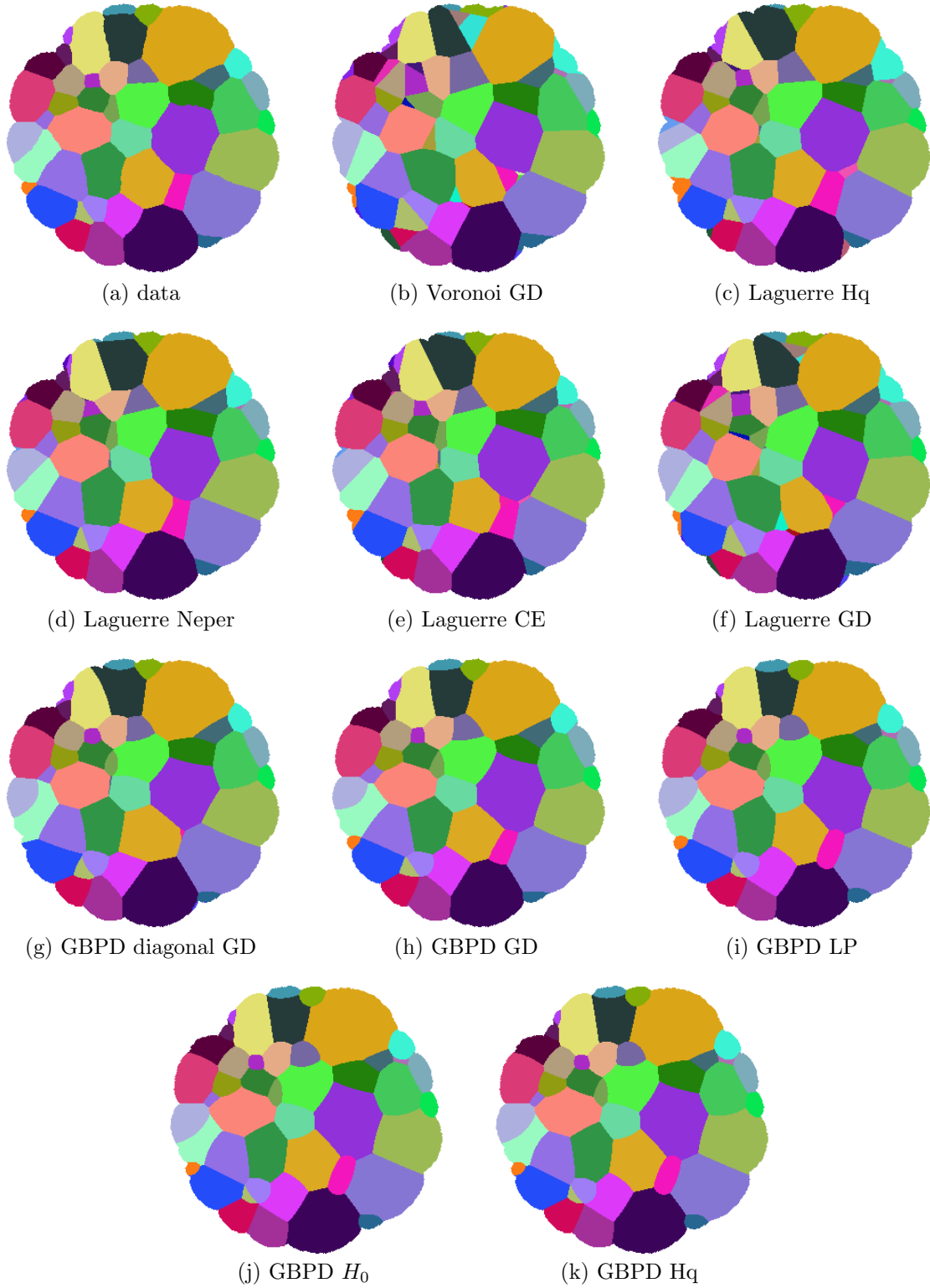


Figure S2: Cross sections of the **AlCuStep20** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using Hq (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i), H_0 (j) and Hq (k).

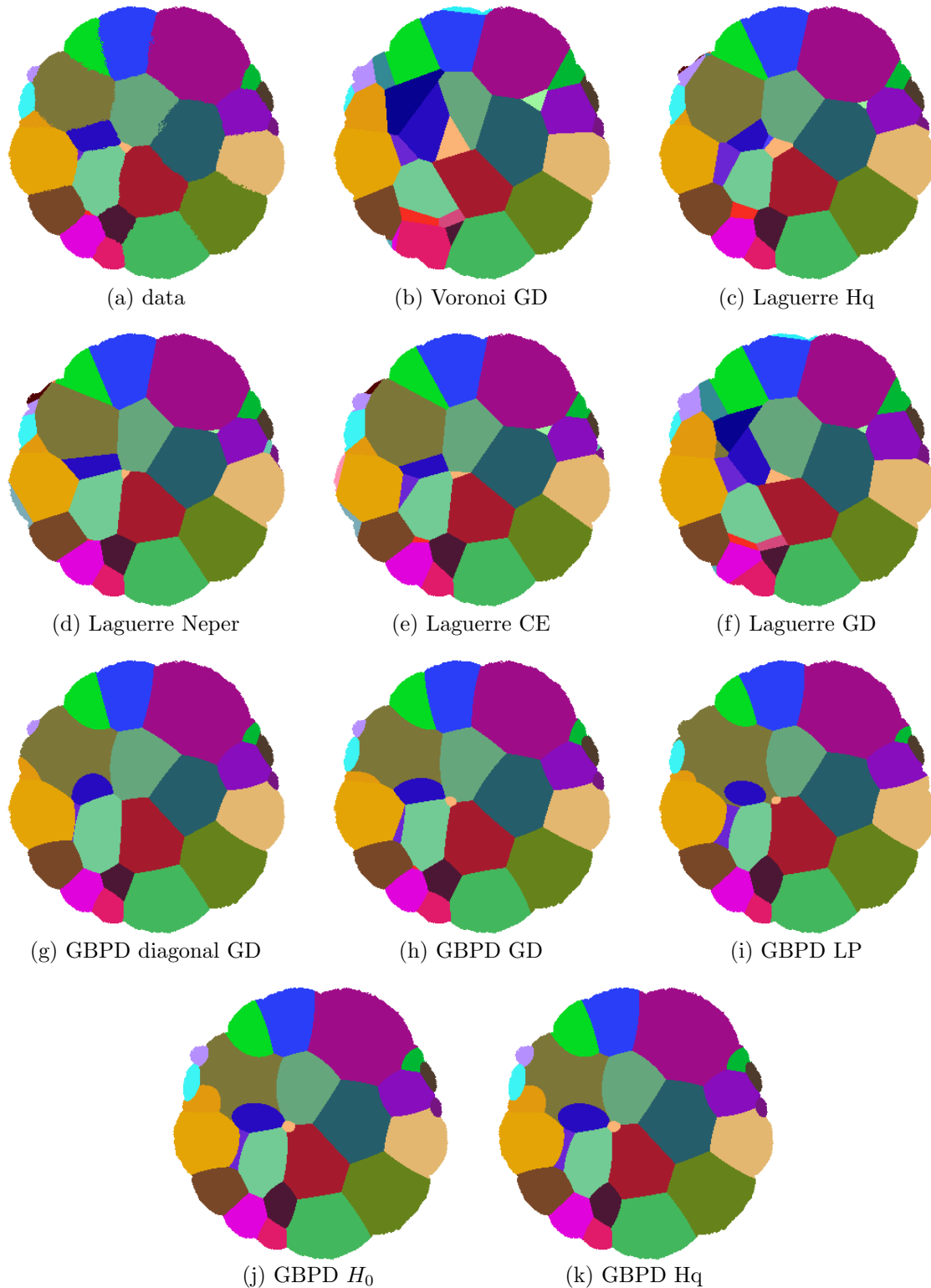


Figure S3: Cross sections of the **AlCuStep60** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using Hq (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i), H_0 (j) and Hq (k).

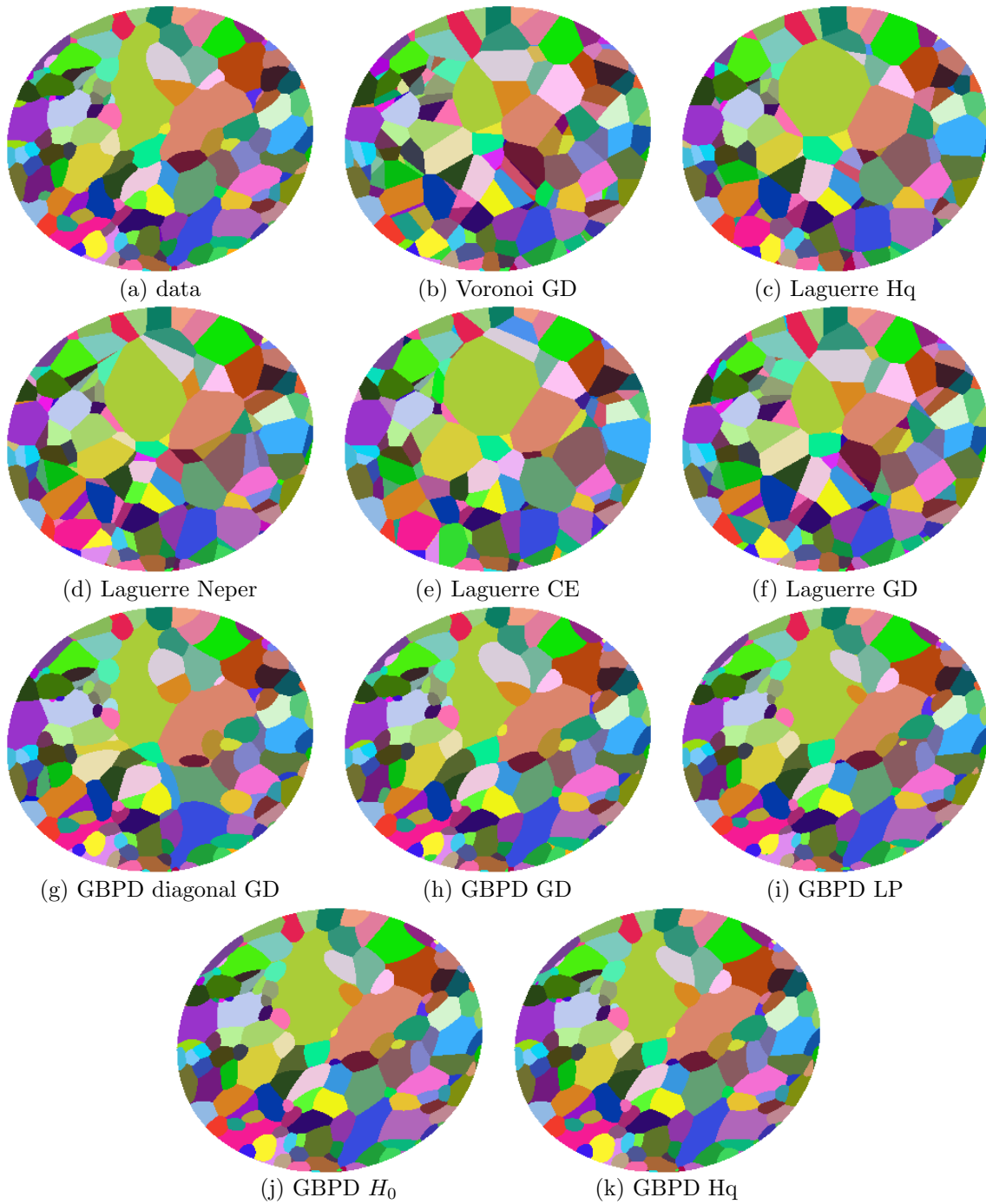


Figure S4: Cross sections of the **PureFeStep0** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using H_q (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i), H_0 (j) and H_q (k).

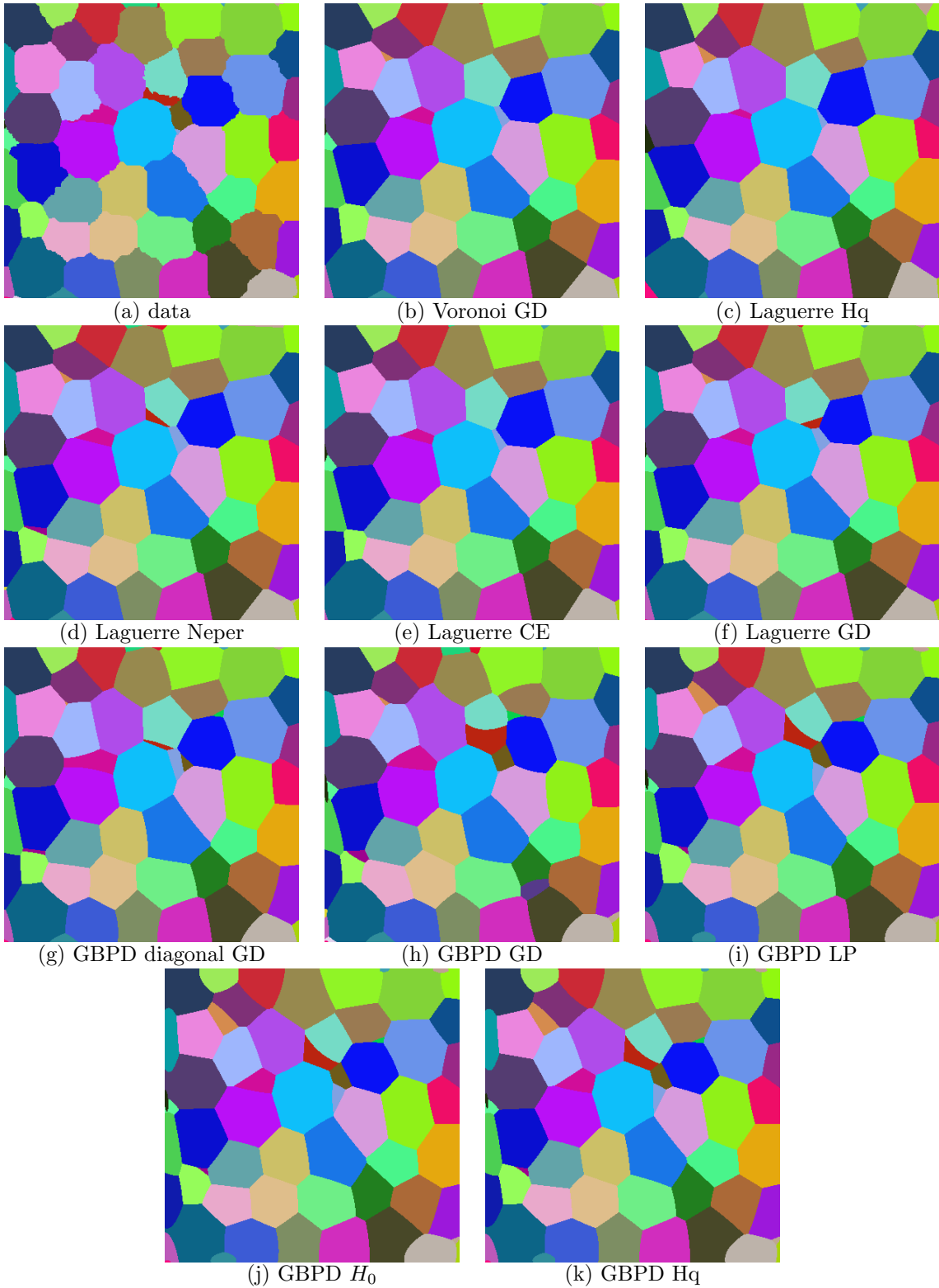


Figure S5: Cross sections of the **Vesuvius** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using Hq (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i), H_0 (j) and Hq (k).

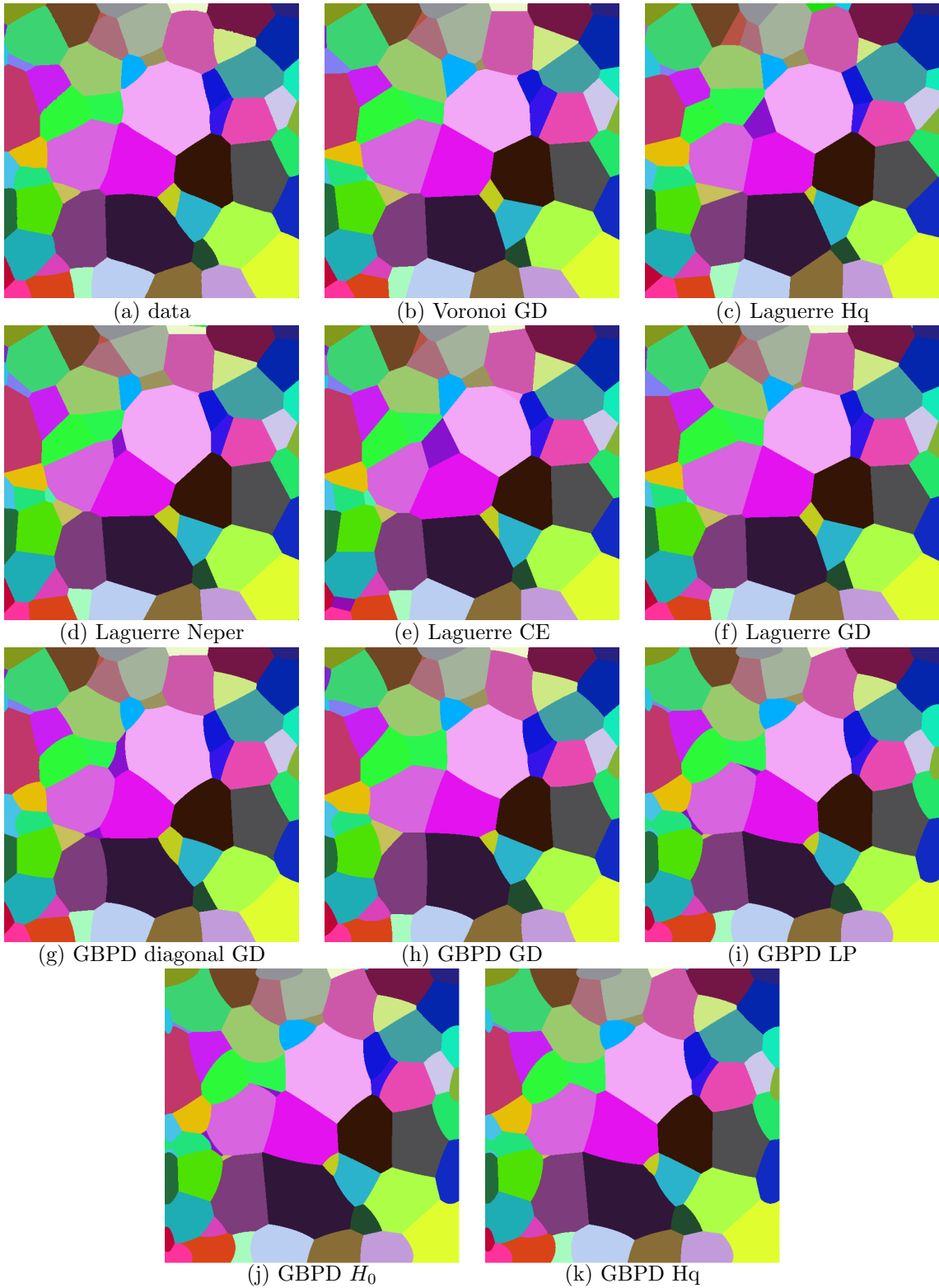


Figure S6: Cross sections of the **WIND** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using Hq (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i), H_0 (j) and Hq (k).

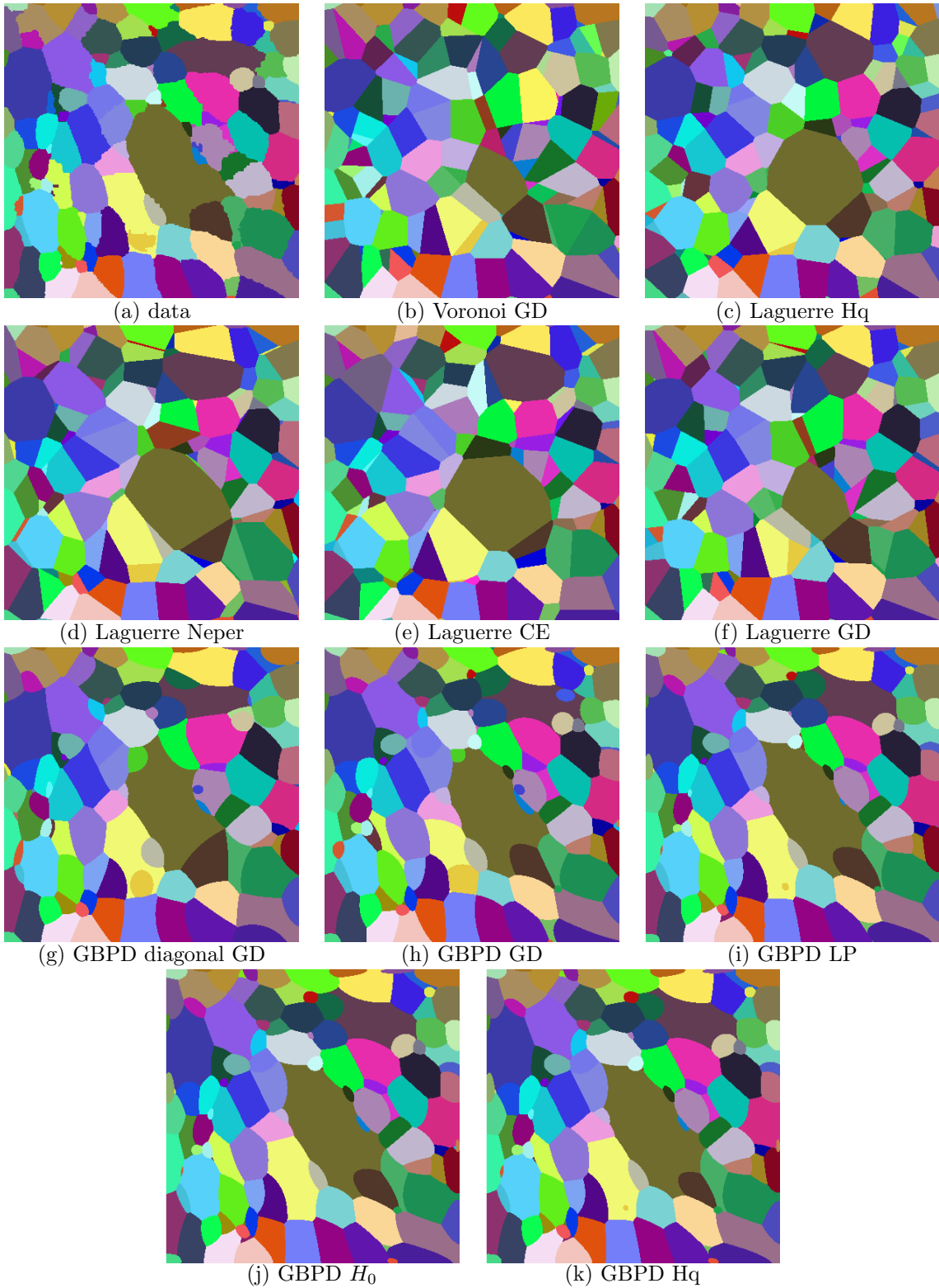


Figure S7: Cross sections of the **Zinc1** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using Hq (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i), H_0 (j) and Hq (k).

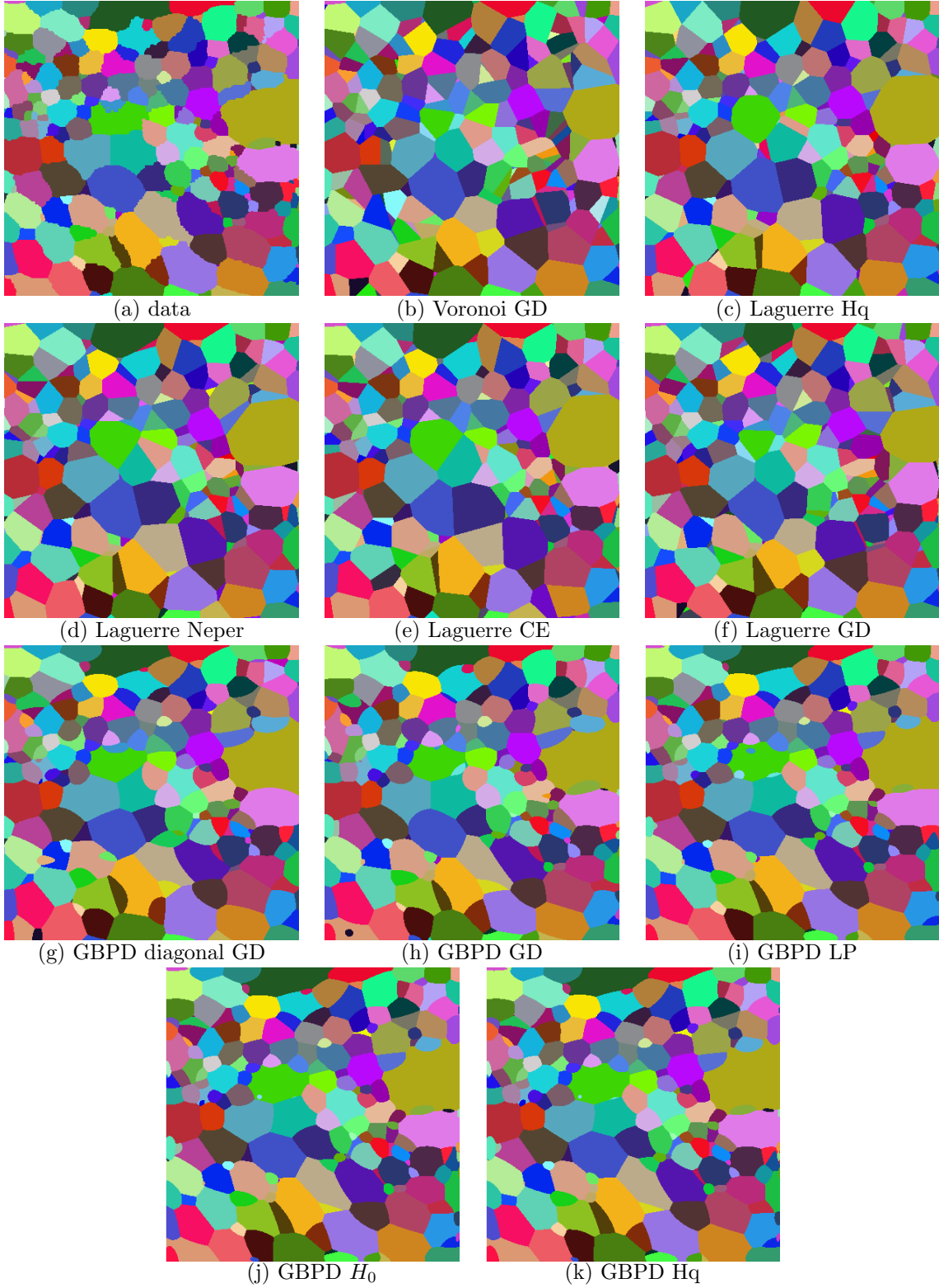


Figure S8: Cross sections of the **Zinc2** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using Hq (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i), H_0 (j) and Hq (k).