# Statistical mechanics in computational geometry

Daniel Duque
ETSIN, UPM

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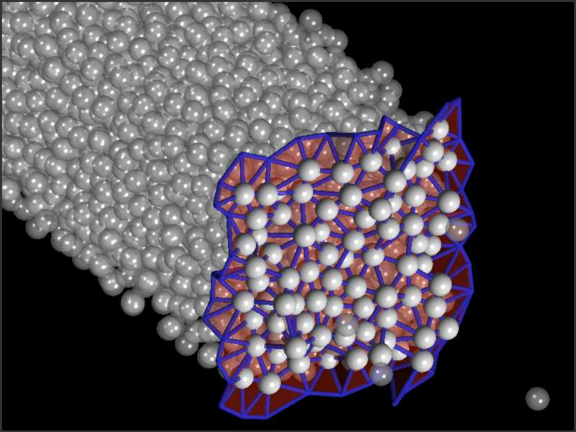
# Motivation

- Notice: in the past, we have applied computational geometry (CG) to statistical mechanics (SM). I.e. the $\alpha$-shapes.
- Today, I'll describe methods *from* SM applied *to* CG.



# The problem

- When discretizing the continuum equations of hydrodynamics using nodes ("particles") one may obtain equations of motion. Direct connection: *Molecular dynamics* No SM, really
- (Actually, interesting SM in the mesoscopic, Brownian regime, but that's not our topic today.)
- How to discretize the equations for some given particles? Some unexpected SM.

# Laws: Navier-Stokes equations

We would be happy to compute these two accurately:
Continuity:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \rho \mathbf{v}$$

Momentum density $\rho v_\alpha$, for each coordinate $\alpha = 1, 2, 3$:

$$\frac{\partial \rho v_\alpha}{\partial t} = -\nabla \cdot \rho v_\alpha \mathbf{v} - \frac{\partial p}{\partial x_\alpha} + \mu \nabla^2 v_\alpha$$

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Use a grid, and finite differences (or finite elements) for equations that are written in this "frame".

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Notice "particles" are fixed here, are just space nodes. There is usually lots of freedom in choosing them (and refining them).

SERG, U. Sheffield

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This calls for a *Lagrangian* approach, and computational methods that will be either *meshless* or have a *moving mesh*.

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In this frame, the equations simplify remarkably. Now, we would be happy just with these.
Lagrangian particles:

$$\frac{D\mathbf{r}}{Dt} = \mathbf{v}$$

Continuity:

$$\frac{DM}{Dt} = 0$$

Momentum:

$$\frac{M}{V}\frac{D\mathbf{v}}{Dt} = -\nabla p + \mu\nabla^2\mathbf{v}.$$

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Given a set of particles with

- positions $\{\mathbf{r}_a\}$,
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$$\frac{D\mathbf{r}_a}{Dt} = \mathbf{v}_a$$

$$\frac{DM_a}{Dt} = 0$$

$$\frac{M_a}{V_a}\frac{D\mathbf{v}_a}{Dt} = -(\nabla p)_a + \mu(\nabla^2 \mathbf{v})_a.$$

# Computing with fluid particles

So, we need to provide expressions for:

- particles' volumes $\{V_a\}$
- pressure gradients $\{(\nabla p)_a\}$
- velocity Laplacians $\{(\nabla^2 \mathbf{v})_a\}$

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- also: we are unable to choose "nice" nodes. Even if we do, they will move around, to who knows where (This is a huge difference with the fixed grid community, such as FEMs).

The standard approach is to introduce a set of weight functions $\{p_a(x)\}$, from which:

$$u(x) = \sum_a u_a p_a(x) \qquad \nabla u(x) = \sum_a u_a \nabla p_a(x) \qquad \ldots$$

(Actually, some quadrature may be needed on top of this.)

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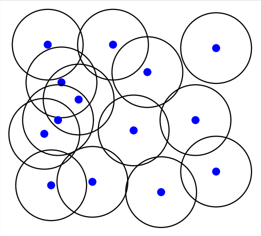
We would like these be satisfied, in some sense, at least. In order of niceness:

- Identically
- For lots of particles ($O(N)$ effort)
- For finer resolution ($O(N^2)$ effort, or worse)

# Popular choices: SPH

$$p_a = \frac{1}{C} \exp[-\beta(x - x_a)^2]$$

| 0-c | 1-c | 2-c | loc | m-free | bound |
|---|---|---|---|---|---|
| | | | | | |



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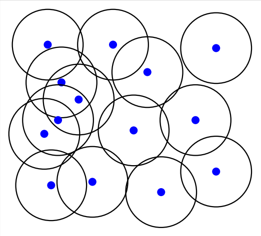

- Quite bad consistency (needs resolution increase to converge), but *very* easy to implement
- Uses: fluids with interfaces, both in science and in animation industry (films, commercials...). Next Limit's Real Flow: LotR, Avatar, Charlie and the Chocolate, Ice Age 1-3,

# Popular choices: SPH-Shepard

$$s_a = \exp[-\beta(x - x_a)^2]$$

$$p_a = \frac{s_a}{Z}$$

$$Z = \sum_a s_a$$

| 0-c | 1-c | 2-c | loc | m-free | bound |
|---|---|---|---|---|---|
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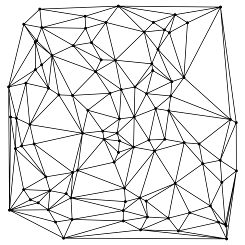
- 0-consistency by construction, the rest is as bad as SPH.

# Popular choices: FEM

$p_a$ = finite elements on Delaunay mesh



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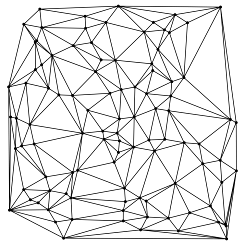
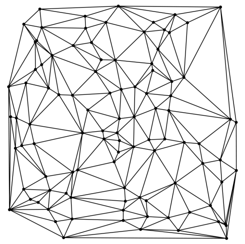


- The very famous Finite Element Method of engineering
- Notice the elements are triangles in 1D, pyramids in 2D, but in the later there are many possible triangulations on which to build them
- The Delaunay lattice is the "best" in many ways: it is the one with more open angles. Plus, its dual is the Voronoi tesselation.

# FEM



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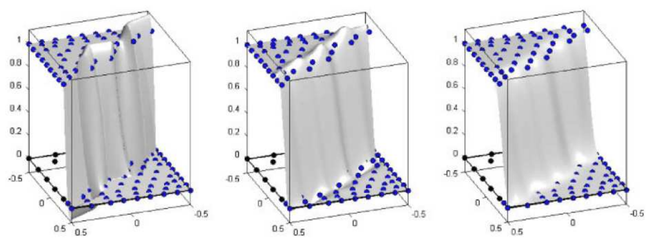
- Exact consistencies by construction.
- But notice: serious stability issues due to fitting.
- In fact, it violates positivity, $p_a < 0$ sometimes.



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FEM seemed really the way to go. But! it *never* converges to the proper $\nabla^2$! (on arbitrary point sets).

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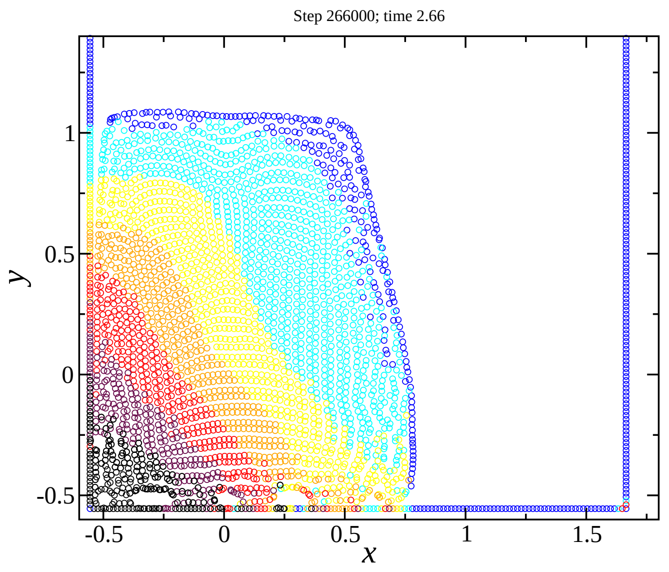
All in all, the FEM can already be used for reasonable results.

# FEM results: dam break



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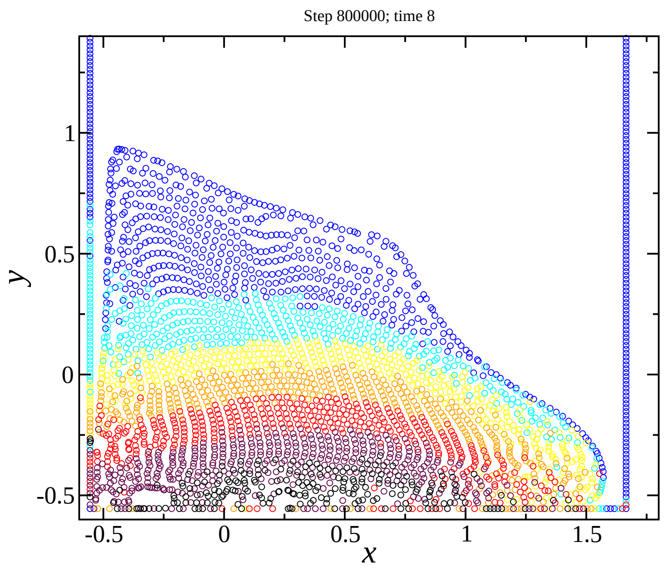

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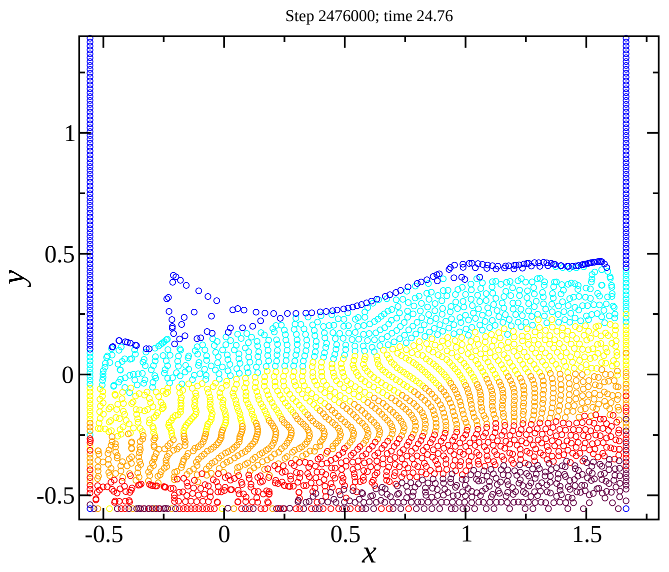

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- Notice: no functional form to the $p_a$. This is both a source of freedom and a computational nuisance.

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Mathematically: extremize

$$\mathcal{L} = \beta \sum p_a(x - x_a)^2 + \alpha \left( \sum p_a - 1 \right) + \lambda \sum p_a(x - x_a)$$

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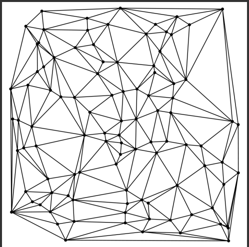

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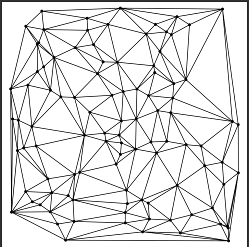

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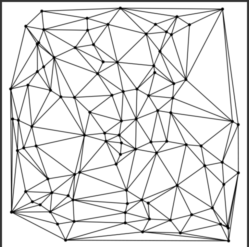

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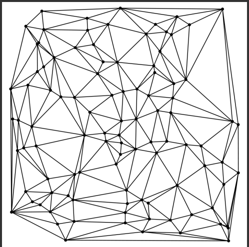
- Amazing or what? (It is to me.)



# LME, continued

- So, this $U$ looks like an energy, doesn't it: $U = \sum p_a(x - x_a)^2$.
- It would be a sort of mean spherical model (all $p_a$ add up to 1), where each "spin" $p_a$ is coupled only to its field $(x - x_a)^2$.

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So, what if we tried "entropy" instead of "energy"?

$$\mathcal{L} = \sum p_a \left(\log p_a - 1\right) + \alpha \left( \sum p_a - 1 \right) + \lambda \sum p_a (x - x_a)$$

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Notice: $S = -\sum p_a \left(\log p_a - 1\right)$, which is maximized.

# LME, continued

Well, in SM the solution to this is well-known:

$$p_a = \frac{1}{Z} \exp\left[-\lambda^*(x - x_a)\right],$$

where $\lambda^*$ is the value:

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Note: this is the physicist's approach to LME. Computing people have an easier time considering this from information theory: $S$ is the information entropy (Shannon's), which reflects how much we know about a system with variables $p_a$. By maximizing it, we choose the least-biased set.

# LME, properties

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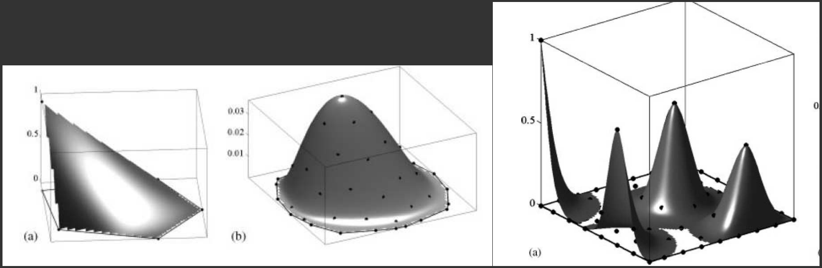
- They automatically die out at the boundary, except for nodes already at the boundary (just like FEM).



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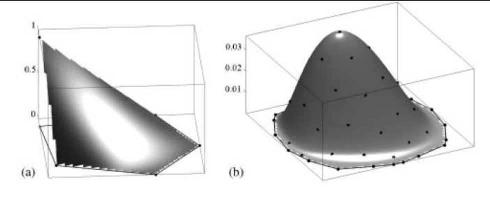


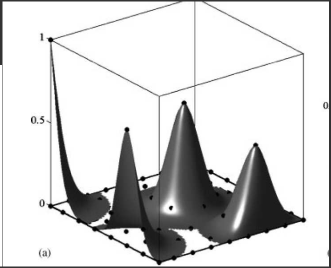


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# Extended LME

The functions are perhaps too wide, so recalling the result by Rajan, we may consider:

$$\begin{aligned}\mathcal{L} &= \beta \sum p_a(x-x_a)^2 + \sum p_a\left(\log p_a - 1\right) + \\ &+ \alpha\left(\sum p_a - 1\right) + \lambda \sum p_a(x-x_a)\end{aligned}$$

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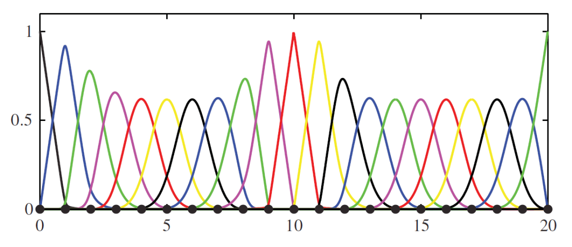
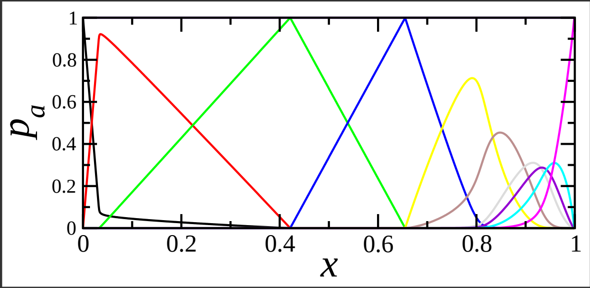
- Pure LEM: $\beta \to 0$. Very hot limit (just entropy)
- Pure Rajan: $\beta \to \infty$. Very cold limit (just energy)
- We can tune $\beta$, even have $\beta = \beta(x)$.

# Extended LME: pictures




Fixed spacing, varying $\beta$




Fixed $\beta$, varying spacing

# LME - SPH connection

Another interesting fact: if we drop 1-cons:

$$\begin{aligned}\mathcal{L} &= \beta \sum p_a (x - x_a)^2 + \sum p_a \left(\log p_a - 1\right) + \\ &+ \alpha \left( \sum p_a - 1 \right),\end{aligned}$$

The solution is just:

$$p_a = \frac{\exp[-\beta (x - x_a)^2]}{Z},$$

SPH-Shepard!

# LME - SPH connection

Another interesting fact: if we drop 1-cons:

$$\begin{aligned}\mathcal{L} &= \beta \sum p_a (x - x_a)^2 + \sum p_a \left(\log p_a - 1\right) + \\ &+ \alpha \left( \sum p_a - 1 \right),\end{aligned}$$

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SPH-Shepard!

I know, this is trivial, but few works bridge these fields: fluids, computational geometry, and statistical physics.

# Limitations of LME

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# Limitations of LME

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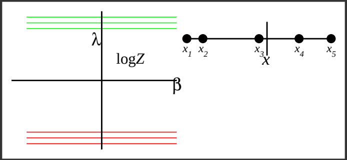
$$\mathcal{L} = \beta \sum p_a (x - x_a)^2 + \dots$$

Clearly, a minimum of $\mathcal{L}$ w.r.t. $\beta$ will likely not be found.
In fact, the minimum will always be $\beta \to \infty$, as we will see next, and FEM will be recovered (which does not have 2-cons!)

# LME's lack of 2-cons

(Argument due to P. Español). The situation is clearer in 1D.




- Low $\lambda < 0$: $Z \approx e^{-\lambda|x-x_1|}$, hence $\log Z \approx -\lambda|x - x_1|$.
- High $\lambda > 0$: $Z \approx e^{\lambda|x-x_5|}$, hence $\log Z \approx \lambda|x - x_5|$.

So, for a fixed $\beta$ we can expect to find a minimum of $\log Z$. This is nothing but the extended LEM.

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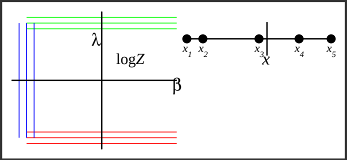



- Low $\beta < 0$: $Z \approx e^{-\beta|x-x_3|^2}$, hence $\log Z \approx -\beta|x-x_3|^2$. OK, thus far. But:
- High $\beta > 0$: $Z \approx e^{-\beta|x-x_3|^2}$, hence $\log Z \approx -\beta|x-x_3|^3$. Disaster.

Hence, the minimum squeezes away towards $\beta \to \infty$!

# Introducing SME

OK, now imagine we had:

$$\log Z \approx \beta(g - |x - x_3|^2),$$

with $g > |x - x_3|^2$?

Now, the minimum would not be at $\beta \to \infty$ any more.

# Introducing SME

OK, now imagine we had:

$$\log Z \approx \beta(g - |x - x_3|^2),$$

with $g > |x - x_3|^2$?
Now, the minimum would not be at $\beta \to \infty$ any more.
But then, of course, our original problem has changed to:

$$\begin{aligned}\mathcal{L} &= \sum p_a (\log p_a - 1) + \alpha \left( \sum p_a - 1 \right) + \\ &+ \lambda \sum p_a (x - x_a) + \beta \left( \sum p_a (x - x_a)^2 - g(x) \right).\end{aligned}$$

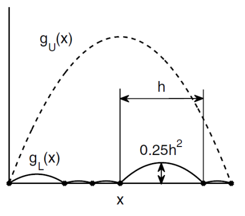
Whose solution is again known from SM:

$$p_a = \frac{1}{Z} \exp\left[ -\lambda^* (x - x_a) - \beta^* \left( (x - x_a)^2 - g(x) \right) \right],$$

$$\lambda^*, \beta^* : \min_{\lambda, \beta} \log Z$$

# SME: the gap

Some inspection of the particular requirement $g > |x - x_3|^2$ shows that in general $g(x)$, called "the gap" should be confined to this region:



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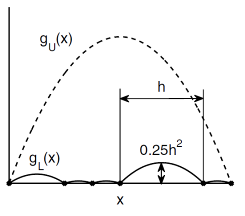
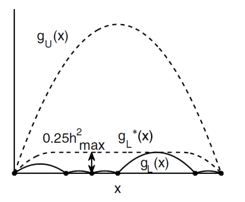



How bad is this? After all, 2-cons is lost . . .

# SME: the gap

Well, not very bad. Consider the following choice

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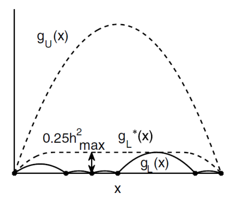


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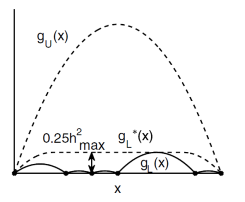


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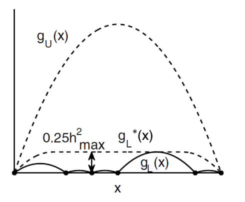


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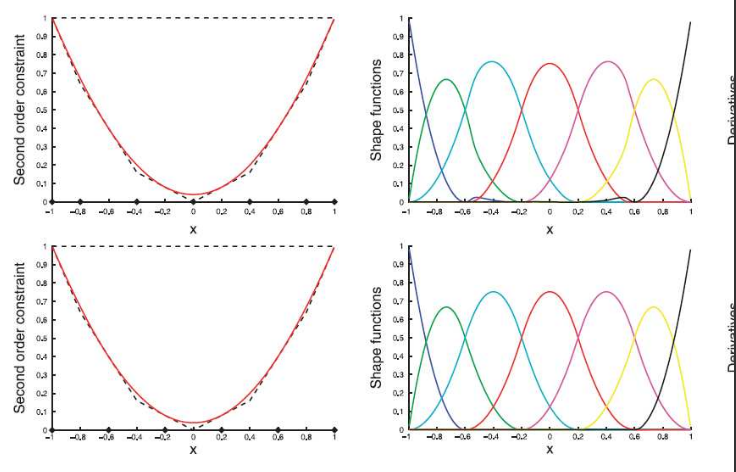
| 0-c | 1-c | 2-c | loc | m-free | bound |
|---|---|---|---|---|---|
| | | | | | |

# SME: some pictures



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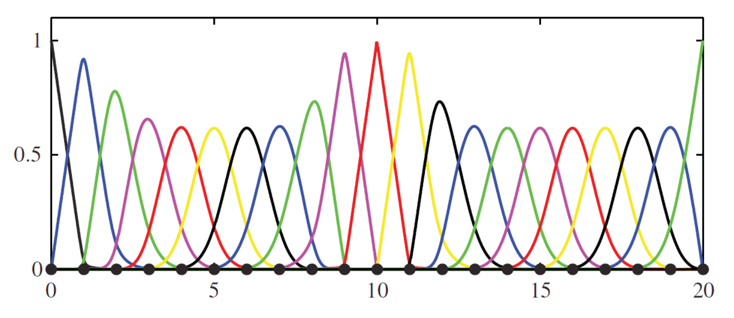


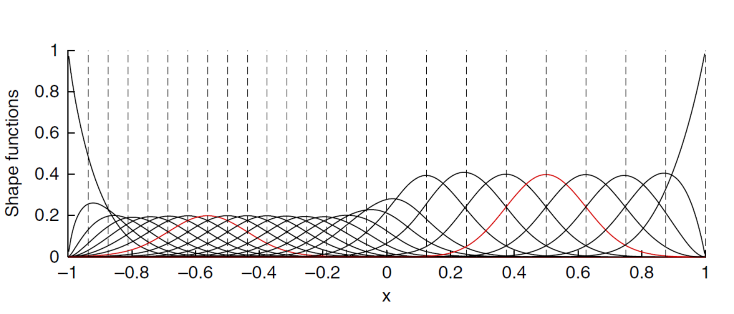

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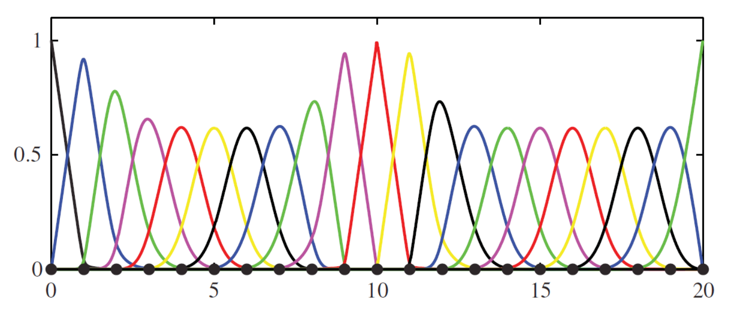


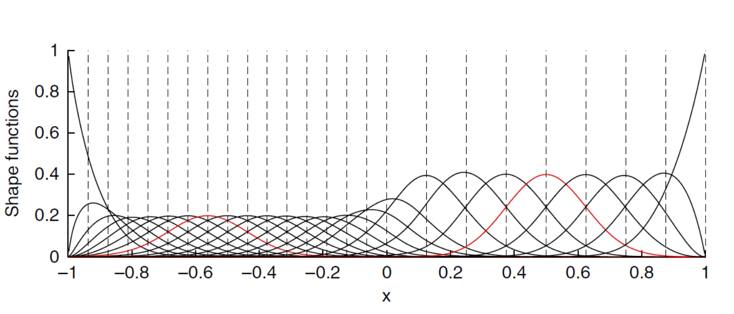

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Is it hard? Not really: a minimization should be performed only at each of the particles (not all $x$), which involves only $\partial_\lambda \log Z$ and $\partial_\sigma \log Z$ (these are quite easy).

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Basically: go ahead, and implement it on a simulation!
Is it hard? Not really: a minimization should be performed only at each of the particles (not all $x$), which involves only $\partial_\lambda \log Z$ and $\partial_\sigma \log Z$ (these are quite easy).
For the derivatives, $\partial^2_{\lambda\lambda} \log Z$ etc are needed, but these are only needed when the minimum has been found. Moreover, some methods (quasi-Newton) are supposed to provide these second derivatives automatically.

# References


- *LME* M. Arroyo and M. Ortiz, *Local maximum-entropy approximation schemes: a seamless bridge between nite elements and meshfree methods*. Int. J. Numer. Meth. Engng 2006; 65:21672202. DOI: 10.1002/nme.1534
- *SME* C.J. Cyron, M. Arroyo, and M. Ortiz, *Smooth, second order, non-negative meshfree approximants selected by maximum entropy*. Int. J. Numer. Meth. Engng 2009; 79:16051632. DOI: 10.1002/nme.2597