Some Lattice-based Scientific Problems, Expressed in Haskell

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1 Introduction

Lazy functional languages haven't, to date, made an enormous impact in scientific computing. Partly, this has to do with performance—codes written in these languages usually run an order of magnitude (or two) slower than imperative codes, which limits their appeal for number-crunching production codes. Apart from that, there is a suspicion that programming without assignments or side-effects is difficult, or restrictive. (Evidently, this isn't the opinion of functional programmers—but maybe there's something peculiar lurking in scientific computation which really can't be *done* easily without assignments.)

This article gives detailed Haskell implementations of three "scientific" algorithms. In order of increasing complexity they are: solution of a partial differential equation by the relaxation method; Monte Carlo simulation of a statistical mechanics system; and a similar simulation of a lattice gauge theory. These problems are taken from theoretical physics—a strongly mathematical discipline. Functional programming also has a very mathematical feel to it. So it shouldn't be too surprising that these problems actually come out rather neatly in a functional language. (Other examples of scientific functional programming can be found in [1, 2, 3]).

Haskell is a relatively new language, put forward as an international standard for functional programming [4, 5, 6]. It is a lazy, pure functional language. Beyond that, the choice of Haskell as a mode of expression in this article is fairly incidental—any lazy functional language would probably have done as well. Having chosen Haskell, however, free use has been made of its more innovative features, including the array and class systems (the latter for achieving overloading, or *ad hoc* polymorphism, in the array manipulation functions we introduce). A fair understanding of Haskell is probably a prerequisite for reading this article. By and large, the "prelude" functions of Haskell will be used without much comment, so a Haskell reference may be necessary.

Full understanding of the problems and algorithms described will require a certain amount of mathematical knowledge—some familiarity with simple partial differential equations, differential operators like the gradient and Laplacian, complex numbers, and a rough grasp of probability distributions. I won't assume any detailed knowledge of the physics behind the problems, but the footnotes fill in some details for those who are interested. Section 2 describes the systems involved and the associated algorithms. The problems are all based on lattices (i.e., grids). They make important use of arrays.

Rather than work directly with standard Haskell arrays, it proved convenient work with a kind of generalised array, with more geometric significance. Section 3.1 describes the approach taken to lattice geometry, and arrays defined on these lattices. The appendices give details of a possible Haskell implementation of the generalised arrays and operations on them. To further illustrate their use there is also an appendix containing some examples based on finite-difference approximations to various differential operators.

I chose to handle the lattices in a rather abstract way, which is why there's a whole section on geometry and generalised arrays. The payoff is that the geometry factors out from the problems in a nice way—the implementations in section 4 make almost no reference to the details of this geometry. Abstraction certainly has dividends, but understanding it also requires some investment of effort. Needless to say, Haskell doesn't *enforce* this level of abstraction. It does enable it.

The implementations of the main algorithms are given in section 4. The paradigm used in each case is one of interacting parallel processes, modelled by lazy lists (streams) representing the output of the processes. Partly this choice can be attributed to the source of funding for this work—the FAST project aims to provide a parallel implementation of annotated functional programs written in essentially this style [7]. Apart from that, the style comes quite naturally and is reasonably efficient in a lazy language, especially for

algorithms with some "locality of reference".

2 Three problems

The choice of problems here reflects strongly an original motivation for this work, namely to "do QCD" in a functional language. *Quantum Chromodynamics*, the theory of the strong nuclear force, is a relativistic quantum field theory. Through a series of mathematical tricks[1], which reduce d-dimensional quantum theories to $(d+1)$-dimensional statistical mechanics problems, it can be expressed as a *lattice gauge theory*. In this form it is amenable to Monte Carlo simulation. In this article, lattice gauge theory will be introduced from a more algorithmic point of view, assuming no particular knowledge of the physical systems involved. First two simpler problems which share some of its features are introduced.

2.1 The 2-dimensional Poisson equation

A fundamental problem in electrostatics is calculation the electric field produced by a given distribution of charges. For an isolated point charge, the electric field is described (in 3-dimensions) by the inverse-square law. For a more complicated system of charges, with non-trivial boundary conditions (for example, the charges may be enclosed in a metal box) there is no simple solution. The electrostatic potential is obtained by solving the associated Poisson equation. For simplicity we describe the two-dimensional case—a third dimension doesn't introduce anything essentially new. The given charge distribution is a function $c(x, y)$ of the coordinates. The electrostatic potential $u(x, y)$ is the solution of the equation

$$(\boldsymbol{\nabla}^2 u)(x, y) = -c(x, y). \tag{1}$$

Having solved for u, the electric field is the gradient $\boldsymbol{F}(x, y) = -(\boldsymbol{\nabla u})(x, y)$.

The most simple-minded approach to solving (1), is to replace it by the finite difference approximation

$$u(x+1, y) + u(x-1, y) + u(x, y+1) + u(x, y-1) - 4u(x, y) = -c(x, y). \tag{2}$$

The coordinates x, y are now integers—assume that they and c have been rescaled to eliminate appearance of the grid spacing parameter. Rearranging (2) as

$$u(x, y) = \frac{1}{4}(\text{sum neighbouring } u \text{ values} + c(x, y)), \tag{3}$$

immediately suggests the simplest iterative algorithm for solving this system. In the *relaxation* algorithm, starting from some initial guess for u, each iteration replaces the value a u at a point by the average value of its neighbours (plus an offset determined by the local charge). Variants differ in whether the u values inserted in the RHS of (3) are those from the previous sweep of the grid (Jacobi relaxation) or whether they are the most recent values, which may include some values already updated in the current sweep (Gauss-Siedel relaxation). The last version has further variations depending on the order in which the grid is traversed—a popular scheme is "red-black relaxation" in which all even sites are visited first, then all odd sites. Straight relaxation is a slow algorithm, but it does form the core update of more powerful methods [12].

2.2 The XY Model

Statistical physics is largely concerned with the study of *phase transitions* in complex systems. Many simplified mathematical models have been introduced which exhibit

[1] The Feynman path-integral formulation of quantum mechanics [8]; analytic continuation to Euclidean space-time (Wick rotation); and Wilson's lattice discretisation of gauge theories [9, 10, 11]

transitions similar to those of physical systems. The *XY model* is an example [13]. It has an unusual transition driven by "condensation of vortex configurations". The kind of model of interest here can be motivated by referring back to the Poisson equation. Equations (1) or (2) can be obtained from variational principles. Solving the system (2) is equivalent to minimising the functional[2]

$$E(u) = \sum_{x,y} \frac{1}{2}\left((u(x+1,y) - u(x,y))^2 + (u(x,y+1) - u(x,y))^2\right) - c(x,y)u(x,y).$$

$E(u)$ is the electrostatic energy of the configuration u; the lowest energy state is, so to speak, the one "preferred by nature"[3].

In statistical physics, states with higher energy are also taken into account. The aim of a simulation is to generate a sequence of configurations of the system, in which the frequency of appearance of a particular configuration u with energy $E(u)$ is weighted by the Boltzmann probability distribution:

$$P(u) \propto \exp(-E(u)/\theta).$$

Here, θ is the temperature of the system[4]. A phase transition generally manifests itself in discontinuous behaviour of some expectation-values as θ passes through a critical value.

In the XY model $u(x,y)$ isn't a single real number. Instead it is a unit-length two-dimensional vector. This vector can be represented as a complex number with unit magnitude. The energy function can then be written as

$$E(u) = -\Re \sum_{x,y} u^*(x,y)u(x+1,y) + u^*(x,y)u(x,y+1),$$

where u^* means complex conjugate of u, and $\Re$ means real part[5]. It isn't difficult to see that E is minimised when every vector is pointing in the same direction as its neighbours. In other words, when *all* vectors point in the same direction.

Some more interesting configurations are also very stable in the XY model. A few of these "vortex" configurations, which are local (rather than absolute) minima of the energy function, are illustracted in figure 1.

Algorithms for generating sequences of configurations with Boltzmann distribution for this type of system resemble relaxation. They are iterative algithms, involving repeated sweeps across the grid, and the update of a single site normally only needs knowledge of the current values at neighbouring sites.

In the *Metropolis* algorithm [14] the update of a site is as follows: choose a candidate new value for the local u by some pseudo-random procedure[6]. Calculate the change in energy, ΔE, which would be produced by replacing the old value of u by the candidate new one (this depends on the state of the neighbouring sites). If ΔE is negative, accept the candidate update. If ΔE is positive, accept the candidate with probability $exp(-\Delta E)$. If the candidate is rejected, retain the original value of u.[7]

[2] Taking the partial derivative of $E(u)$ with respect to $u(x,y)$, for some fixed (x,y), and setting the result to zero, recovers equation (2).

[3] The squared terms in E are discrete difference approximations to the squared electric field, $\boldsymbol{F}^2$.

[4] As $\theta \to 0$, states with energy above the minimum are exponentially suppressed, and the simulation yields the ground state with probability approaching 1—an observation underlying the *simulated annealing* method of minimisation.

[5] Alternatively, each vector can be parametrised by its angle from some fixed direction. This gives the equivalent expression $E(u) = -\sum \cos(\theta(x+1,y) - \theta(x,y)) + \cos(\theta(x,y+1) - \theta(x,y))$

[6] The procedure should give equal probabilities for rotating the vector by $+\delta$ and $-\delta$, for all angles δ. Also it should be "ergodic"—by combining some sequence of allowed updates it must be possible to get from any state to any other

[7] The proof of this algorithm is omitted. The crux is to show that, when the probability of a

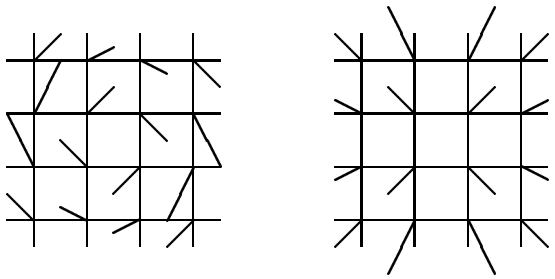


Figure 1: Vortex configurations of the XY model

2.3 Lattice gauge theory

This section describes the so-called $U(1)$ lattice gauge theory[8], associated with QED (*Quantum Electrodynamics*). QED is closely related to QCD; the modifications needed to go to QCD are outlined at the end of the section. The main difference between $U(1)$ gauge

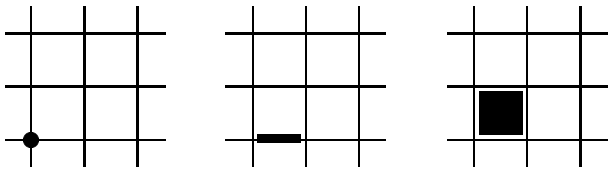


Figure 2: Some elementary cells of a lattice.

theory and the XY model is geometric. In the XY model the variables u are associated with the *sites* of the lattice. The energy function (2.2) is a sum over the *links* of the lattice—it involves multiplying together the values of the variables at the ends of each link.

In gauge theory the variables are associated with the links of the lattice, and the energy function is computed on the next-higher dimension cells of the lattice—the elementary squares, or *plaquettes* (figure 2).

We can associate a group element (a unit-magnitude complex number) U_P with any path P in the lattice by multiplying together the link variables along the path. The energy function is

$$E(u) = - \sum_{P \in plaquettes} \Re(U_P)$$

where *plaquettes* is the set of elementary plaquette-paths in the lattice.[9]

The Metropolis algorithm can be carried over from the XY model. The local update is identical. The difference lies in how the neighbouring values which effect the local contribution to the energy are collected. In the XY model, the local contribution to the

system state is given by the Boltzmann formula, the expected frequency of transitions (produced by the algorithm) from any state A to any other state B is the same as that from B to A ("detailed balance") so that the Boltzmann distribution represents equilibrium.

[8] $U(1)$ is the group of unit magnitude complex numbers, with complex multiplication as the product

[9] In the XY model energy, one of the factors in the link product has to by conjugated. In gauge theory, variables associated with links which have negative incidence on the plaquette are conjugated. This will be illustrated more fully in the next two sections.

energy was determined by the values of site variables at neighbouring sites. In gauge theory it is determined by link variables on the "staples" illustrated (in the 3-dimensional case) in figure 3.

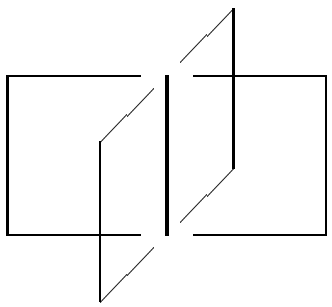


Figure 3: Surrounding links, contributing to the energy of the central one.

For real physics, the lattice should be four dimensional. The procedure described here simulates the "gauge-particles" of a theory (photons or gluons). It doesn't take account of matter particles. The modification required to handle QCD rather than QED is that the link variables should be elements in the group, $SU(3)$, of unit-determinant, 3×3, unitary matrices, rather than simply unit-magnitude complex numbers.

3 Generalised Arrays

A straightforward way to store the values of, for example, the potential function u in section 2.1 is in a Haskell array. This works well, provided the lattice is a regular grid and its extent is rectangular. It works less well in the case of lattice gauge theory (section 2.3). There the variables naturally live on the links of the lattice. One can still use an array indexed by lattice sites, with an extra dimension taking values in $1, \ldots, d$ to access the d links rooted at each site (d is the dimension of the lattice). This is quite clumsy.

We can think of the sites of a lattice as the 0-dimensional cells of the lattice, the links as the 1-dimensional cells, the plaquettes as 2-dimensional cells, and so on. Occurrence of variables which naturally live on cells with dimension higher than 0 is more common than one might initially suppose. Even in the Poisson equation the electric field, which is the gradient of the potential, sits most naturally on the links of the lattice. The field in the x-direction is associated with links in that direction; its value is just the difference of the potential at the two ends of its link. In the XY model the vortex configurations illustrated in figure 1 are centred on the plaquettes of the distribution—one can define a function which counts the density of vortices in a general configuration, and this function resides naturally on the plaquettes of the lattice. As explained in section 2.3, the energy function of a gauge theory also "lives" on the plaquettes of a lattice.

This suggests that it may be useful to generalise our model of an array so that it is defined on an arbitrary (not necessarily recangular) lattice, and that the index space of a particular array can be cells of that lattice of arbitrary (fixed) dimension. This generalised kind of array will be called a "form"[10].

The lattice itself is no longer thought of just as a set of connected sites, but as a "cell complex" containing cells of all dimensionality up to that of the lattice itself.

3.1 Cells, lattices and forms

This section assumes some knowledge of the Haskell class system. The standard prelude defines, for example, the class `Ix`. All types which can be used as index types for an array belong to this class. A type specification involving type variables may be preceded by an assertion that some of those variables belong to class `Ix`. Array operations like the array subscripting operator `(!)` (which, by the way, is an ordinary infix function—not special syntax) are *overloaded* to apply to all instances of `Ix`.

We need a Haskell class `Cell` which parallels the index class `Ix` associated with ordinary arrays. Two type constructors `Lattice` and `Form` go with this class. They construct the following types[11]:

```
(Cell a) => Lattice a
(Cell a) => Form a b
```

The latter is directly analogous to the ordinary Haskell `Array` constructor—`Form a b` is the type of a form with cell-type `a` and elements of type `b`. `Lattice a` is the type of a data structure describing a lattice with cells of type `a`. It takes over the role of the bounds pair for an ordinary array.

To make this more concrete, a possible instance of the `Cell` class, suitable for handling 2-dimensional rectangular lattices, is

```
data Cell2d = Cell2d0 (Int, Int)      |
```

[10] This terminology is motivated by an analogy between this kind of array and the p-forms of differential geometry [15]. It might have been more accurate to adopt the term "cochain" from algebraic topology[16]. But I thought of "form" first, and it's shorter.

[11] The `(Cell a) =>` prefix asserts that the type `a` must be an instance of class `Cell`.

```
        Cell2d1 (Int, Int) Int |
        Cell2d2 (Int, Int)
```

which can represent a site, link or plaquette of the lattice[12]. The numeric fields are the cell coordinates, and in the 1-cell case, the link direction. The cell type alone doesn't define the lattice shape. We need at least to know the size of a rectangular lattice, and besides that, the "edge conditions" have to be specified—the lattice may have a boundary at the edges, or be connected cyclically, etc. We will assume that someone has provided a function such as

```
torus2d :: Int -> Int -> Lattice Cell2d
```

which takes the width and height of the lattice as parameters, and returns an instance of an abstract data type representing (in this example, let's say) a periodic lattice of the specified size. A possible implementation of `torus2d` is given in appendix C. Now, we can start building forms. The function analogous to the ordinary Haskell `array` is

```
form :: (Cell a) => Lattice a -> Int -> [Assoc a b] -> Form a b
```

This constructs a form from an "association list". The first parameter is the lattice on which the form is to be defined; the second is the "rank", r, of the form—that is, the dimension of the cells on which it is defined; the third is an association list completely analogous to the corresponding argument of `array`—a list of pairs associating each cell of dimension r in the lattice with a value. As a mundane example, the expression

```
form l 1 [c := 0.0 | c <- cells l 1]
```

is 1-form with value 0.0 on each link of lattice `l`.

```
cells :: (Cell a) => Lattice a -> Int -> [a]
```

is analogous to `range`, returning a list of all cells of a specified dimension in the given lattice. Ultimately, the following operations on forms will also be needed

```
accumForm :: (Cell a) => Lattice a -> Int -> [Assoc a b] -> Form a [b]
lattice   :: (Cell a) => Form a b -> Lattice a
rank      :: (Cell a) => Form a b -> Int
(!#)      :: (Cell a) => Form a b -> a -> b

(//#)     :: (Cell a) => Form a b -> [Assoc a b] -> Form a b

listForm  :: (Cell a) => (Lattice a) -> Int -> [b] -> Form a b

fassocs   :: (Cell a) => Form a b -> [Assoc a b]
findices  :: (Cell a) => Form a b -> [a]
felems    :: (Cell a) => Form a b -> [b]

fmap      :: (Cell a) => (b -> c) -> Form a b -> Form a c
fmapi     :: (Cell a) => (a -> b -> c) -> Form a b -> Form a c
fzipWith  :: (Cell a) => (b -> c -> d) -> Form a b -> Form a c
                                                   -> Form a d
```

[12] `Form` and `Lattice` types will be treated, in this section at least, as abstract types. There doesn't seem to be much advantage in treating the cell types themselves as abstract—it's convenient to have access to the constructors, for referring to an element of the lattice at known coordinates

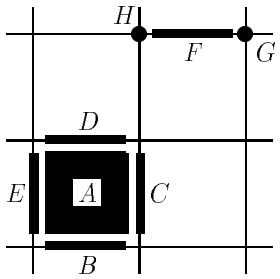
Most of these are fairly self-explanatory generalisations of similarly-named Haskell prelude functions. A possible implementation of them is given in appendix A. Use of those definitions requires an instance of the cell class. An example instance is given in appendicix B.

`(!#)` is the infix subscripting operation on a form, so if `a` is a form and `c` is a cell of the right type and dimension, `a !# c` is the corresponding element of `a`. `lattice` and `rank` generalise the standard `bounds` function, returning the lattice and rank of a given form. `accumForm` is similar to `form` but the requirement of one association for every cell is relaxed—the result is a form containing for each cell a list of all values the association list bound to that cell[13]. `fmap` is a straightforward mapping function. `fmapi` is similar, but the mapping function is passed an extra argument, the cell on which the function map is being applied. `fzipWith` is similar to the `zipWith` function on lists. It takes two conforming forms and produces a third by applying the zipping function at each cell.

3.2 Lattice topology

The final and most interesting ingredient is the `boundary` operation.

A powerful way of representing the topology of a cell complex is through its *incidence function*. This is a function I from pairs of cells to the set $\{-1, 0, +1\}$. It's value is non-zero only when the cell pair is of the form $(c^{(r)}, c^{(r-1)})$, where $c^{(r)}$ is an r-dimensional cell, and $c^{(r-1)}$ is an $(r-1)$-dimensional cell, *and $c^{(r-1)}$ is on the boundary of $c^{(r)}$*. When it is non-zero, its value is $+1$ or -1 according to whether $c^{(r-1)}$ is positively or negatively oriented on the boundary of $c^{(r)}$. Orientation is easier to grasp through pictures than by formal definition—see figure 4. In the figure the conventions are adopted that the links



$$
\begin{aligned}
I(A,B) &= +1 \\
I(A,C) &= +1 \\
I(A,D) &= -1 \\
I(A,E) &= -1 \\
I(F,H) &= -1 \\
I(F,G) &= +1 \\
I(A,F) &= 0 \\
I(B,H) &= 0
\end{aligned}
$$

Figure 4: Example values of the incidence function on a 2d lattice.

are directed from left to right or from bottom to top, and the boundary of a plaquette is oriented anti-clockwise around the square. So, for example, link B has positive incidence on plaquette A, because it follows the direction of the boundary path, whereas D has negative incidence because it is directed left to right while the top boundary of A goes right to left. For the incidence of a site on a link, the convention is that it is positive if the link is directed in to of the site, and negative if it is directed out of the site[14].

Now the `boundary` function,

```
boundary  :: (Cell a, Num b) => Lattice a -> a -> [Assoc a b],
```

[13] This doesn't quite correspond with the related operation on arrays in the prelude. This was just a matter of personal taste

[14] Reversing any of these conventions on orientation may change local signs in the incidence function, but *not* the final, scalar results of computations.

applied to an r-cell `c` returns the list of $(r-1)$-cells on the boundary of that cell, paired with the incidence function of the boundary cell on `c`. Taking examples in figure 4:

```
boundary l A = [B := 1, C := 1, D := -1, E := -1]
boundary l F = [H := -1, G := 1]
boundary l H = []
```

where `l` is the associated lattice data structure. The result for H is empty, because by convention 0-cells have no boundary. (There is no huge significance in the choice of `Assoc` pairs as the result of `boundary`. In principle, any type capable of representing a cell and a numeric object would do.) Appendix C shows how a particular lattice topology can be set up—defining an instance of the `boundary` function.

The `boundary` operation probably looks a bit contrived at first sight. Rather than diving into the main applications in the next section, it may be useful to see what kind of thing it is good for. For readers familiar with the differential operators involved, the examples in appendix D will probably help. Here we just record a couple of functions used there, which are also needed in the next section (these don't actually use the `boundary` operation).

First, a function which "contracts" a form on an association list containing cells and values of the same type:

```
cntrct :: (Cell a, Num b) => Form a b -> [Assoc a b] -> b
cntrct a c = sum [v * (a !# j) | j := v <- c]
```

(This is a sort of scalar product between a form and an association list).

Second, `mltply` multiplies all values in an association list by its first argument.

```
mltply :: (Cell a, Num b) => b -> [Assoc a b] -> [Assoc a b]
mltply m ivs = [i := m * v | i := v <- ivs]
```

4 Form-based implementation of the three algorithms

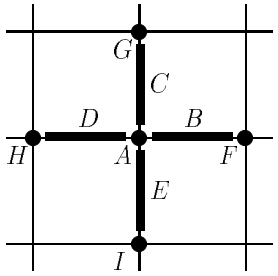
4.1 Accessing neighbours

Consider the function

```
neighbours :: (Cell a, Num b) =>
              Lattice a -> Int -> Form a [[Assoc a b]]
neighbours l r = accumForm l r
  [j := mltply v (if v == (-1) then reverse b else b)
                 | b      <- [boundary l i | i <- cells l (r + 1)],
                   j := v <- b]
```

`mltply` was defined in section 3.2[15]. If `r` is zero (for example) `b` is instantiated to the boundary of each link in the lattice in term. Link B in figure 5 would yield (up to a possible re-ordering of lists)

```
b = [A := -1, F :=  1]
```



$$
\begin{aligned}
I(B,A) &= -1 \\
I(C,A) &= -1 \\
I(D,A) &= +1 \\
I(E,A) &= +1 \\
I(B,F) &= +1 \\
I(C,G) &= +1 \\
I(D,H) &= -1 \\
I(E,I) &= -1
\end{aligned}
$$

Figure 5: Collection of 0-cells neighbouring A.

This gives rise to the terms

```
[ ..., A := [A :=  1, F := -1],
       F := [F :=  1, A := -1], ...]
```

in the outer list comprehension (the list in the second association is obtained by reversal and multiplication by -1). After the application of `accumForm`, the value at site A will be (again, up to possible re-ordering of lists)

```
[[A :=  1, F := -1],
 [A :=  1, G := -1],
 [A :=  1, H := -1],
 [A :=  1, I := -1]]
```

The form produced by `neighbours` contains some redundant information (probably all that was really needed was the identities of F, G, H and I). However, the definition here is generalised to produce forms of neighbours for arbitrary-dimension lattice cells, which will be useful later.

As a first application of `neighbours`, the Laplacian operator of appendix D could be reimplemented by

[15] The application of `reverse` in the definition of `neighbours` is no more than cosmetic for the examples given here, because none of them is sensitive to the list ordering in the result of `boundary`, but see footnote 21.

```
laplacian a = fmap (cntrct a . concat) (neighbours l r)
              where l = lattice a
                    r = rank a
```

where `cntrct` was defined in section 3.2.

As a second application, we define a mapping function for the 0-cell case, which operates on a pair-wise, nearest-neighbour basis

```
nns :: (Cell a) => (a -> a -> b -> c) -> Form a b -> Form a [c]
nns f a = fmapi (\i ivss ->
            [f i j (a !# j) | ivs <- ivss, j := v <- ivs, v < 0])
                (neighbours l 0)
          where l = lattice a
```

This exploits the knowledge that neighbours proper appear with a negative value in the association list, filtering out occurrences of the "destination" cell itself. The mapping function is passed the destination cell, the "source" cell and the value of the original form at the source cell. In the example above we would have

```
(nns f a) !# A = [f A F (a !# F), f A G (a !# G),
                  f A H (a !# H), f A I (a !# I)]
```

4.2 Poisson equation relaxation.

With the geometry well sorted out, we can do an application. Define a data type which captures the local state in a relaxation calculation:

```
type Obs    = Float

data State  = Interior Float Obs | Boundary Obs

siteObs :: State -> Obs
siteObs (Interior _  u) = u
siteObs (Boundary    u) = u

siteTrans :: State -> [Obs] -> State
siteTrans (Interior c _) nbs =
           Interior c ((sum nbs + c) / fromIntegral (length nbs))
siteTrans  b             _   = b
```

There are two types of site: normal sites on the "interior" of the lattice, and those on some designated boundary (which could be empty)[16]. Sites on the interior have a local charge density and a potential value. Those on the boundary just have a potential value, which will remain a fixed throughout the iteration. The function `siteObs` extracts the "observable", i.e. the potential, from a `State` variable. `siteTrans` performs the update of equation (3) on the interior sites and leaves boundary sites unchanged. It is passed the old value of the site and a list of potential values at nearest neighbours.

The history of a single site can be regarded as a stream of `State` values[17]. The site evolves through application of a transition function which depends on the (changing) environment of the site. This pattern of evolution can be captured through the function[18]

[16] This grid "boundary" shouldn't be confused with the cell `boundary` operation

[17] By definition, a "stream" is an infinite list

[18] `process` can also be implemented by `scanl`. Note the lazy pattern-match on the last parameter of `process`. This laziness is required for the implementations below.

```
process :: (s -> e -> s) -> s -> [e] -> [s]
process trans st ~(env : envs) = st : process trans (trans st env) envs
```

In the present case the current environment is a list of neighbour potential values, and the last argument to `process` will be a stream of such lists—the history of the environment.

The result of the computation will be a 0-form of lists of `State` values, defining the history of the whole lattice. Suppose we are given this form and need to calculate the 0-form of environments from it. This can be done by

```
env :: (Cell a) => Form a [State] -> Form a [[Obs]]
env = fmap transpose . nns (\_ _ -> map siteObs)
```

The application of `nns`, in which the mapping function extracts a stream of potential values from the stream of `State` values, gives a form containing a list of streams of neighbour histories. Mapping `transpose` over it turns these into streams of neighbour lists. These are just what `siteTrans` needs as its argument. So the implementation of relaxation is

```
evolve :: Form Cell2d State -> Form Cell2d [State]
evolve init = x where x = fzipWith (process siteTrans) init e
                      e = env x
```

The argument is a 0-form of initial states (`fzipWith` is defined to pick up the lattice from its first array parameter).

This code implements Jacobi relaxation. More general schemes, like Gauss-Siedel, can easily be implemented in the same framework. Suppose a site A has site B as a neighbour. The scheme above calculates the new value at A in terms of the previous generation value at B. To calculate the value of A in terms of the *latest* value of B, we should look one place forward in the history of B—in other words the B stream should be tailed before feeding it into the environment of A. To organise this, it is convenient to attribute a colour to each site. If the colour of B, say, is less than the colour A, A is updated in terms of the latest value of B. Otherwise it is updated in terms of the previous generation value of B. The function `env` is changed to

```
env = fmap transpose .
        nns (\i j -> map siteObs .
                     if colour j < colour i then tail else id)
```

Red-black Relaxation in 2 dimensions can be implemented by

```
colour (Cell2d0 (x, y)) = (x + y) `mod` 2
```

4.3 XY model simulation

To describe the local state in an XY model simulation, the `State` data type is changed in the following way:

```
type Obs    = Complex Float

data State = MkStat Float [Float] Obs

siteObs (MkStat _ _ s) = s

siteTrans (MkStat theta rans spin) neighbs = MkStat theta rans'' spin'
  where
```

```
    (cand, rans')   = metroCand rans spin
    eDiff           = deltaE neighbs spin cand
    (spin', rans'') = metroChoice spin cand (eDiff / theta) rans'
```

The fields in the `State` record are respectively the temperature, an infinite list of randoms, and the local value of u (sometimes called the "spin"). Each site must hold an *independent* stream of random numbers. Creating the random number streams is part of initialisation—I'll omit details here[19].

As explained in section 2.2, the Metropolis update has three stages—choose a candidate update; calculate the change it would make to the system's energy; decide on the basis of this whether to accept the candidate or retain the old value at the site. The details are:

```
-- Energy difference between two spin states.
deltaE neighbs s s' = - real (conjugate (sum neighbs) * (s' - s))
                      where real (x :+ _) = x

-- Canditate new spin for Metropolis update.
metroCand (r : rans) old = (exp (0 :+ delta) * old, rans)
                           where delta = max_delta * (2 * r - 1)

-- Metropolis choice.  Inputs are old and candidate new variable,
-- energy difference of configurations, and a list of randoms.
metroChoice _   new ediff  rans       | ediff < 0 = (new, rans)
metroChoice old new ediff (r : rans') =
  (if accept then new else old, rans') where accept = r < exp (- ediff)
```

`metroCand` returns a unit-magnitude 2-vector which differs from the one input by rotation through a random angle in the range [−`max_delta`, +`max_delta`].

The remainder of the code is identical to that in the previous section[20].

4.4 Lattice gauge theory simulation

The 1-form analogue of `nns` is

```
staples :: (Cell a, Num b) => (a -> [(a, b, c)] -> d) ->
                              Form a c -> Form a [d]
staples f a =
  fmapi (\i ivss ->
         [f i [(j, v, a !# j) | j := v <- snip i ivs] | ivs <- ivss])
                                                  (neighbours l r)
  where l           = lattice a
        r           = rank a
        snip i ivs  = tail (rotate (\(j := _) -> j == i) ivs)
        rotate p xs = b ++ f where (f, b) = break p xs
```

[19] There are various approaches to getting independent streams of pseudo-random numbers. If the basic generator has a long enough cycle, simply taking independent seed values (perhaps chosen by a different generator) may be acceptable. Alternatively, here are various "leapfrog" schemes available [17], which are quite elegant. I actually used a leapfrogged 64-bit linear congruential generator.

[20] The Red-black variant is preferred—in this case the "Jacobi" version would actually be invalid because neighbouring sites connected by the energy function would be updated "concurrently", and localised calculation of the energy change would be erroneous.

The mapping function has a more complicated specification here. There are two reasons for this. First, each adjacent plaquette defines several (in a cubic lattice, three) neighbours to a given link, whereas an adjacent link only defined a single neighbour to a given site. Second, orientation information is irrelevant to sites, but important for links (links are directed; sites aren't). The mapping function again takes the "destination" cell as it's first argument. Its second argument is a list. The items in this list correspond to the links in a single staple (see figure 3). Each item is a tuple containing the coordinate (cell) of the link, it's orientation relative to the destination cell ($+1$ or -1 depending on whether it points in the same or the opposite direction around the boundary of the plaquette), and the value held at the link[21].

Now, the definition of `env` is changed to

```
env = fmap transpose .
      staples (\i lss ->
                (map product . transpose)
                [((if v == -1 then map conjugate else id) .
                  map siteObs .
                  (if colour j < colour i then tail else id)) ls |
                                                (j, v, ls) <- lss])
```

The list comprehension pre-processes the streams of states associated with the links on a given staple. In contrast to the previous version, variables are conjugated here if they have negative orientation relative to the destination link (in the XY model, this conjugation was also necessary, but was deferred to `deltaE`). The resulting streams are zipped together by the `transpose`, `map product` pipe, to produce a stream of products around the staple.

Colouring is slightly more complicated than before. We have to ensure that no two links lying on the same plaquette have the same colour (see footnote 20). For a 4 dimensional cubic array a suitable definition might be[22]

```
colour (Cell4d1 (t, x, y, z) d) = 4 * ((t + x + y + z) `mod` 2) + d.
```

Finally, the local state and updating can be lifted verbatim from the XY model, except that `deltaE` is simplified to

```
deltaE neighbs s s' = - real (sum neighbs * (s' - s))
                      where real (x :+ _) = x
```

because the conjugation was already done in `env`. The top-level evolution is unchanged from section 4.2 (the type specification of `evolve` has to be altered slightly). One might want to change some names: the "site" prefixes ought to become "link" or, more generically, "cell".

[21] The function `snip` cuts out the destination link from the list of links around the plaquette. In `nns`, this was done by a filter in the list comprehension. The same method could be used here. But that would loose information on the order of links around the staple (assuming that the implementation of `boundary` returned the links around a plaquette in path-order to start with). This information is preserved by the device of rotating the list so the destination link is at the front, and tailing it. If the gauge group was non-Abelian (as it is in full QCD, but not in the simplified case described here) this path-ordering information would be important.

[22] To save space, this article doesn't define an implementation of 4-dimensional geometry. The modifications necessary to the 2-dimensional case given in the appendices are reasonably straightforward.

5 Discussion

The algorithms described involve state transition in an essential way, but it's doubtful whether their description would have been any clearer in terms of variables and assignments. The explicit representation of sequences as infinite lists seems just as natural.

The implementations in section 4 create an "array of streams". An alternative approach is to create a "stream of arrays", in which each update is performed on the whole lattice to create a new global state. It only involves minor changes to the implementation to create such a stream of arrays directly. Alternatively one can feed the results of the given implementation to a pipeline of `felems`, `transpose` and `map (listForm l r)` to produce a list of arrays. There are some advantages to the "array of streams" approach (apart from the fact that it models process-parallelism). Some existing Haskell implementations don't handle array accesses very efficiently[23], and in this approach the array operations are confined to an initial stage where the streams are "tied together". In the "stream of arrays" approach array operations are needed in all updates. On the other hand it does seem more natural to have a list of arrays when it comes to processing the data (the set of configurations) generated by a simulation.

In any case, once the ideas about lattices and arrays in section 3.1 are absorbed, implementation of the three algorithms is very straightforward. It was worth the effort of doing the geometry carefully, for the level of generality it gave in the implementations. For example, apart from the definition of `colour`, the modifications made to the XY model simulation in section 4.4 to encompass lattice gauge theory didn't actually invalidate the code as an implementation of the XY simulation—the final version works for systems with variables defined on arbitrary dimension cells of an arbitrary dimension lattice (given an appropriate instance of the `Cell` class). Achieving this level of abstraction depended on both ordinary (parametric) polymorphism and overloading.

The price one pays for this generality is that while all the programs given in this article are executable, they run much too slowly to be regarded as production simulation programs. Unless functional compilers make rapid progress, it's difficult to imagine that they can be competitive in this rôle in the immediate future. Presumably the functional programs themselves could be optimised to gain significant factors in speed (and efficiency of memory utilisation). No major efforts were made in this direction, after a few early attempts, which were thwarted by difficulty in understanding the behaviour (in terms of execution speed and memory utilisation) of the programs. Programmers who need speed are usually happy to invest some effort in optimising their own codes. They often do it better than compilers, provided they have a reasonably accurate idea of what goes on during execution. Unfortunately, it's relatively difficult to form such a mental model for a lazy functional language. Good profiling tools may make the job easier[18].

As they stand, though, the programs capture the essence of the algorithms in a way that a production FORTRAN code probably never could. At the very least, programs like this must have a rôle in specification or prototyping.

[23] It seems that functional programming and parallel programming share this characteristic—if "array" is interpretted as distributed data in the parallel case. Locality of reference is a helpful feature of an algorithm for both paradigms

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[16] **** Choose some book on Algebraic topology ****

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[18] **** Something on profiling ****

A The "form" library

```
module Lattice (Cell (cellEnum, cellArray, cellAccum, dimension),
                Lattice (MkLattice),
                Form,
                cells, boundary,
                form, accumForm, lattice, rank, (!#), (//#),
                listForm, fassocs, findices, felems,
                fmap, fmapi, fzipWith) where

-- The underlying technology of lattices and their forms...
-- This parallels the 'PreludeArray' section for arrays.

infixl 9 !#
infixl 9 //#

-- The 'Cell' class is the analogue of the 'Ix' class in 'PreludeCore'.

class (Eq a) => Cell a where
  cellEnum  :: Int -> [a] -> [a]
  cellArray :: Int -> [a] -> [Assoc a b] -> a -> b
  cellAccum :: Int -> [a] -> [Assoc a b] -> a -> [b]
  dimension :: a -> Int


-- First field in 'Lattice' defines extent of the complex, where required.
-- Second field is the 'boundary' function for the complex.

data (Cell a) => Lattice a = MkLattice (Int -> [a]) (a -> [Assoc a Int])
data (Cell a) => Form a b  = MkForm (Lattice a) Int (a -> b)

cells     :: (Cell a) => Lattice a -> Int -> [a]
boundary  :: (Cell a, Num b) => Lattice a -> a -> [Assoc a b]


form      :: (Cell a) => Lattice a -> Int -> [Assoc a b] -> Form a b
accumForm :: (Cell a) => Lattice a -> Int -> [Assoc a b] -> Form a [b]
lattice   :: (Cell a) => Form a b -> Lattice a
rank      :: (Cell a) => Form a b -> Int
(!#)      :: (Cell a) => Form a b -> a -> b

(//#)     :: (Cell a) => Form a b -> [Assoc a b] -> Form a b

listForm  :: (Cell a) => (Lattice a) -> Int -> [b] -> Form a b

fassocs   :: (Cell a) => Form a b -> [Assoc a b]
findices  :: (Cell a) => Form a b -> [a]
felems    :: (Cell a) => Form a b -> [b]

fmap      :: (Cell a) => (b -> c) -> Form a b -> Form a c
fmapi     :: (Cell a) => (a -> b -> c) -> Form a b -> Form a c
```

```
fzipWith  :: (Cell a) => (b -> c -> d) -> Form a b -> Form a c
                                                  -> Form a d

-- 'Lattice' primitives...

cells    (MkLattice cls _) r = cellEnum r (cls r)
boundary (MkLattice _ bdy) i = [j := fromIntegral s | j := s <- bdy i]

-- 'Form' primitives...

form      l@(MkLattice cls _) r ivs = MkForm l r (cellArray r (cls r) ivs)
accumForm l@(MkLattice cls _) r ivs = MkForm l r (cellAccum r (cls r) ivs)
lattice (MkForm l _ _) = l
rank    (MkForm _ r _) = r
(!#)    (MkForm _ _ d) = d

-- Higher level operations on Forms...

a //# us   = form (lattice a) (rank a)
             ([i := a !# i | i <- findices a \\ [i | i := _ <- us]] ++ us)

listForm l r vs = form l r (zipWith (:=) (cells l r) vs)

fassocs  a = [i := a !# i | i <- cells (lattice a) (rank a)]
findices a = cells (lattice a) (rank a)
felems   a = [a !# i | i <- findices a]

fmap   f a = form l r [i := f (a !# i) | i <- cells l r]
             where l = lattice a
                   r = rank    a

fmapi  f a = form l r [i := f i (a !# i) | i <- cells l r]
             where l = lattice a
                   r = rank    a

fzipWith f a b = form l r [i := f (a !# i) (b !# i) | i <- cells l r]
                 where l = lattice a
                       r = rank    a
```

B An example instance of the "Cell" class

```
module Cell2d (Cell2d (Cell2d0, Cell2d1, Cell2d2)) where

-- A 'Cell' instance suitable for representing cells in a 2d grid.

import Lattice (Cell (cellEnum, cellArray, cellAccum))

data Cell2d = Cell2d0 (Int, Int)     |
              Cell2d1 (Int, Int) Int |
              Cell2d2 (Int, Int)         deriving (Text)
```

```
ix0 (Cell2d0 i)        = i
ix1 (Cell2d1 (x, y) d) = (x, y, d)
ix2 (Cell2d2 i)        = i

bd0 [c1, c2]    = (ix0 c1, ix0 c2)
bd1 [c1, c2]    = (ix1 c1, ix1 c2)
bd2 [c1, c2]    = (ix2 c1, ix2 c2)

cell0 i         = Cell2d0 i
cell1 (x, y, d) = Cell2d1 (x,y) d
cell2 i         = Cell2d2 i

instance Cell Cell2d where

  cellEnum r cls =
    case r of
      0 -> [cell0 i | i <- range (bd0 cls)]
      1 -> [cell1 i | i <- range (bd1 cls)]
      2 -> [cell2 i | i <- range (bd2 cls)]

  cellArray r cls ivs =
    case r of
      0 -> (array (bd0 cls) [ix0 i := v | i := v <- ivs] !) . ix0
      1 -> (array (bd1 cls) [ix1 i := v | i := v <- ivs] !) . ix1
      2 -> (array (bd2 cls) [ix2 i := v | i := v <- ivs] !) . ix2

  cellAccum r cls ivs =
    case r of
      0 -> (accumArray (flip (:)) [] (bd0 cls) [ix0 i := v | i := v <- ivs] !)
             . ix0
      1 -> (accumArray (flip (:)) [] (bd1 cls) [ix1 i := v | i := v <- ivs] !)
             . ix1
      2 -> (accumArray (flip (:)) [] (bd2 cls) [ix2 i := v | i := v <- ivs] !)
             . ix2
```

C Example definition of lattice geometry

```
module Torus2d (torus2d) where

-- 'torus2d' returns an object of type 'Lattice Cell2d' implementing
-- a 2 dimensional grid with periodic boundary conditions.

import Lattice (Cell (cellEnum, cellArray, cellAccum), Lattice (MkLattice))

import Cell2d (Cell2d (Cell2d0, Cell2d1, Cell2d2))

torus2d :: Int -> Int -> Lattice Cell2d
torus2d lx ly = MkLattice (cls lx ly) (bdy lx ly)

-- Lattice bounds, specified by smallest and largest cell of each dimension:
```

```
cls lx ly 0 = [Cell2d0 (0, 0),   Cell2d0 (lx - 1, ly - 1)]
cls lx ly 1 = [Cell2d1 (0, 0) 0, Cell2d1 (lx - 1, ly - 1) 1]
cls lx ly 2 = [Cell2d2 (0, 0),   Cell2d2 (lx - 1, ly - 1)]

-- Lattice topology (cell boundary):

bdy _ _ (Cell2d0 _) = []

bdy lx ly (Cell2d1 (x, y) d) =
  [Cell2d0 (x, y) :=  -1,
   Cell2d0 (case d of
              0 -> ((x + 1) `mod` lx, y)
              1 -> (x, (y + 1) `mod` ly)) := 1]

bdy lx ly (Cell2d2 (x, y)) =
  [Cell2d1 (x, y) 0 :=  1,
   Cell2d1 ((x + 1) `mod` lx, y) 1  :=  1,
   Cell2d1 (x, (y + 1) `mod` ly) 0  := -1,
   Cell2d1 (x, y) 1 := -1]
```

D Derivatives

Example 1: the gradient

An example alluded to several times is the gradient ∇a of a 0-form a (i.e., a function defined on the sites of a lattice). The gradient can be implemented by

```
gradient :: (Cell a, Num b) => Form a b -> Form a b
gradient a = form l 1 [i := cntrct a (boundary l i) | i <- cells l 1]
             where l = lattice a
```

To see how this works, refer back the figure 4. The result on link F is given by[24]

```
    cntrct a (boundary l F)
  = cntrct a [H := -1, G := 1]
  = ((-1) * (a !# H)) + (1 * (a !# G))
  = (a !# G) - (a !# H)
```

which is, as advertised, a plausible lattice approximation to the gradient $\partial a/\partial x$ of `a` on this x-directed link (if x is the horizontal coordinate in the figure).

Example 2: the divergence

Another operator familiar from differential vector calculus is the divergence, $\nabla.\boldsymbol{a}$, of a vector field $\boldsymbol{a}$. Interpret the vector field as a 1-form. First introduce the function

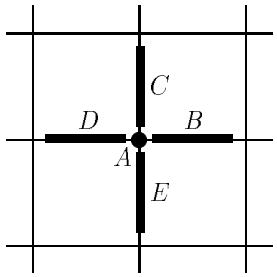
```
bndry :: (Cell a, Num b) => Lattice a -> [Assoc a b] -> [Assoc a b]
bndry l ivs = concat [mltply v (boundary l i) | i := v <- ivs]
```

Given an association list, `bndry` returns another which is a concatenation of the boundaries of all cells in the original list, each multiplied by the value associated with the cell[25]. Divergence can be implemented by

[24] The order of the list returned by `boundary` hasn't been defined. It doesn't effect the result of any of the calculations defined here. The explicit examples choose some order arbitrarily.

[25] This probably seems like an odd concept. It's inspired by the boundary operation on chains in homology—an association list is something like a chain, as the manipulations in appendix E hint.

```
divergence :: (Cell a, Num b) => Form a b -> Form a b
divergence a = (fmap sum . accumForm l 0 . bndry l . fassocs) a
               where l = lattice a
```



$$\begin{aligned} I(B,A) &= -1 \\ I(C,A) &= -1 \\ I(D,A) &= +1 \\ I(E,A) &= +1 \end{aligned}$$

Figure 6: Calculation of the "divergence".

Referring to figure 6, the only links on whose boundary the site A lies are B, C, D and E. So, restricting attention to associations of A in the concatenated boundary list, yields

```
[ ..., A := (a !# B) * (-1), ..., A := (a !# C) * (-1),
  ..., A := (a !# D) * 1, ..., A := (a !# E) * 1, ...]
```

Applying `accumForm` collects together all values associated with the same site into a 0-Form. Up to a possible re-ordering of the list, the value of this form at a site A will be

```
[(a !# B) * (-1), (a !# C) * (-1), (a !# D) * 1,(a !# E) * 1]
```

Mapping `sum` over this form

```
((a !# D) - (a !# B)) + ((a !# E) - (a !# C))
```

Apart from a slightly annoying overall sign, this is what one would expect as a lattice approximation to

$$\frac{\partial a_x}{\partial x} + \frac{\partial a_y}{\partial y}.$$

Example 3: general exterior and interior derivatives, and curl

The operations `gradient` and `divergence` generalise immediately to give approximations to the general exterior and interior derivatives:

```
exterior :: (Cell a, Num b) => Form a b -> Form a b
exterior a = form l r [i := cntrct a (boundary l i) | i <- cells l r]
             where l = lattice a
                   r = rank a + 1

interior :: (Cell a, Num b) => Form a b -> Form a b
interior a = (fmap sum . accumForm l r . bndry l . fassocs) a
             where l = lattice a
                   r = rank a - 1
```

As another concrete example, referring to figure 4 again, the exterior derivative of a 1-form `a` is a 2-form. Evaluated on plaquette A the result is

```
((a !# C) - (a !# E)) - ((a !# D) - (a !# B))
```

which is recognisably a lattice approximation to

$$\frac{\partial a_y}{\partial x} - \frac{\partial a_x}{\partial y}$$

i.e., a component of the curl, $\boldsymbol{\nabla} \times \boldsymbol{a}$ (which is an antisymmetric 2-tensor in general).

Example 4: Laplacians

A generalised Laplacian operator can be implemented by

```
laplacian :: (Cell a, Num b) => Form a b -> Form a b
laplacian = interior . exterior
```

The Laplacian maps an r-form to another r-form. Its effect on a 0-form will be familiar—up to an overall sign[26] the result of applying it to u is given at site (x, y) by the LHS of equation (2).

On a 1-form the result at a particular link is a certain sum of signed values taken from the links on the plaquettes surrounding that link, illustrated in figure 3.

To end this section we re-emphasize that the implementations given here are independent of the details of the lattice shape. Any sensible lattice topology can be encoded in the `boundary` function, which is why it is a powerful concept.

E Why the Laplacian has the wrong sign

If one adopts the shorthand

∂c	$\sim$	`bndry 1` c
(a, c)	$\sim$	`cntrct` a c
$*a$	$\sim$	`fassocs` a
$*c$	$\sim$	`fmap sum . accumForm l r` c
$\mathbf{d}a$	$\sim$	`exterior` a
δa	$\sim$	`interior` a

where a is a form and c an association list, which take values in some numeric type, the following algebraic identities are satisfied

$$\begin{aligned} (\mathbf{d}a, c) &= (a, \partial c) \\ \delta a &= *\partial * a \\ ** a &= a \\ (a, ** c) &= (a, c) \\ (*c, *a) &= (a, c). \end{aligned}$$

Now, for any a

$$\begin{aligned} (\delta \mathbf{d}a, *a) &= (a, *\delta \mathbf{d}a) \\ &= (a, \partial * \mathbf{d}a) \\ &= (\mathbf{d}a, *\mathbf{d}a) \end{aligned}$$

This is a sum of squares. So $\delta\mathbf{d}$, adopted as the definition of the Laplacian above, is a positive semi-definite operator. The conventional definition of the Laplacian is negative.

[26] This a peculiarity of our definition. Appendix E sheds some light on it.