b) Formal Closure

It is straightforward to give a formal "solution" of the closure problem. We illustrate this with a simple generic stochastic dynamical equation

$$\partial_t a(x,t) = K(x,t;a) + f(x,t) \qquad (0)$$

where $K(x,t;a)$ is a functional of the field and $f(x,t)$ is a random noise with mean zero:

$$\langle f(x,t) \rangle = 0$$

A deterministic equation with random initial conditions fits into this framework, where the initial condition

$$a(x,t_0) = a_0(x), \quad \langle a_0(x) \rangle = 0$$

is achieved by an impulsive force at time $t = t_0$:

$$f(x,t) = a_0(x)\,\delta(t-t_0).$$

If this equation is coarse-grained, one obtains

$$\partial_t \bar{a}_\ell(x,t) = \bar{K}_\ell(x,t;a) + \bar{f}_\ell(x,t)$$

where

$$\bar{K}_\ell(x,t;a) = (G_\ell * K)(x,t;a)$$

is no longer closed in terms of $\bar{a}_\ell$, depending on the fine-grained field $a(x,t)$. By linearity, $\langle \bar{f}_\ell \rangle = 0$.

Introduce the complementary field

$$a_\ell'(x,t) = a(x,t) - \overline{a}_\ell(x,t)$$

which represents the small-scale component at length-scales less than ℓ. It is easy to see that

$$\partial_t a_\ell'(x,t) = K_\ell'(x,t;a) + f_\ell'(x,t)$$

with $K_\ell' = K - \overline{K}_\ell$, $f_\ell' = f_\ell - \overline{f}_\ell$. Of course, $\langle f_\ell' \rangle = 0$.

We may write the large-scale and small-scale equations as

$$\begin{cases} \partial_t \overline{a}_\ell(x,t) = \overline{K}_\ell(x,t;\overline{a}_\ell + a_\ell') + \overline{f}_\ell(x,t) & (1) \\ \partial_t a_\ell'(x,t) = K_\ell'(x,t;\overline{a}_\ell + a_\ell') + f_\ell'(x,t) & (2) \end{cases}$$

which illustrates the coupling.

Now, suppose given a particular solution $\overline{a}_\ell, a_\ell'$ of the above system (1), (2). We may solve eq. (2) formally as

$$a_\ell'(x,t) = A_\ell'(x,t;\overline{a}_\ell, f_\ell')$$

where A_ℓ' is a causal functional of $\overline{a}_\ell, f_\ell'$, i.e. depending only on the past history

$$\{\overline{a}_\ell(x,s), f_\ell'(x,s), s<t\}$$

of these two fields.

The substitution of this formal solution of (2) back into (1) yields the equation

$$(3) \quad \partial_t \overline{a}_\ell(x,t) = \overline{K}_\ell(x,t;\overline{a}_\ell + A'_\ell[\overline{a}_\ell, f'_\ell]) + \overline{f}_\ell(x,t)$$

which is now formally closed, since it depends only upon $\overline{a}_\ell$ itself and the noise terms $\overline{f}_\ell, f'_\ell$. We call (3) the <u>formal closure equation</u> for $\overline{a}_\ell$. It is convenient to introduce a deterministic part

$$\overline{K}_\ell^*(x,t;\overline{a}_\ell) = \langle \overline{K}_\ell(x,t;\overline{a}_\ell + A'_\ell[\overline{a}_\ell, f'_\ell]) \rangle$$

where the average is over f (or f'_ℓ) and a random term

$$f_\ell^*(x,t;\overline{a}_\ell, f'_\ell) = \overline{K}_\ell(x,t;\overline{a}_\ell + A'_\ell[\overline{a}_\ell, f'_\ell]) - \overline{K}_\ell^*(x,t;\overline{a}_\ell)$$

so that $\langle f_\ell^* \rangle = 0$. We thus obtain, finally,

$$\boxed{(3^*) \quad \partial_t \overline{a}_\ell(x,t) = \overline{K}_\ell^*(x,t;\overline{a}_\ell) + \overline{f}_\ell(x,t) + \overline{f}_\ell^*(x,t)}$$

There is <u>memory</u> or <u>history-dependence</u> in both $\overline{K}_\ell^*$ and $\overline{f}_\ell^*$, which both depend upon $\{\overline{a}_\ell(s), s<t\}$. The new noise term $\overline{f}_\ell^*$ is thus also <u>multiplicative</u> in character, since it is functionally dependent on $\overline{a}_\ell$. Such equations are called <u>generalized Langevin equations</u>.

Example: Consider the linear Langevin equations

$$\begin{cases} \dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{y} + \mathbf{f}(t) \\ \dot{\mathbf{y}} = \mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{y} + \mathbf{g}(t) \end{cases}$$

where $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$ and $\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}$ are $n \times n$, $n \times m$, $m \times n$ and $m \times m$ real matrices, resp. $\mathbf{f} \in \mathbb{R}^n$, $\mathbf{g} \in \mathbb{R}^m$ are Gaussian white-noise random vectors with covariances

$$\langle \mathbf{f}(t)\mathbf{f}^T(t') \rangle = \mathbf{F}\,\delta(t-t')$$
$$\langle \mathbf{g}(t)\mathbf{g}^T(t') \rangle = \mathbf{G}\,\delta(t-t')$$

for $\mathbf{F}, \mathbf{G}$ positive $n \times n$, $m \times m$ matrices, resp.

In this case, one can show that $\mathbf{x}$ satisfies the generalized Langevin equation

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \int_{-\infty}^{t} ds\, \mathbf{K}(t-s)\,\mathbf{x}(s) + \mathbf{f}(t) + \mathbf{f}^*(t)$$

where

$$\mathbf{K}(\tau) = \mathbf{B}e^{\mathbf{D}\tau}\mathbf{C}$$

and $\mathbf{f}^*(t)$ is a Gaussian vector random process with covariance

$$\mathbf{F}^*(t,t') = \langle \mathbf{f}^*(t)[\mathbf{f}^*(t')]^T \rangle$$
$$= \int_{-\infty}^{t \wedge t'} ds\, \mathbf{B}e^{\mathbf{D}(t-s)}\mathbf{G}e^{\mathbf{D}^*(t'-s)}\mathbf{B}^*$$

The formal closure is, unfortunately, useless for direct application. In fact, it is just a very cumbersome reformulation of the starting equation (0)! It is usually far easier to numerically solve (0) rather than (3) or (3*).

However, the formal closure is <u>conceptually</u> useful. It shows the "correct" form of the closure equation, which, in general, involves long-time memory and induced noise from interactions of resolved and unresolved scales.

The formal closure procedure is also useful as the point of departure for approximation procedures. E.g. see

G. L. Eyink, "Turbulence Noise," J. Stat. Phys. <u>83</u> 955–1019 (1996)

in the context of turbulent fluids, or

C. W. Gardiner, "Quantum noise and quantum Langevin equations," IBM J. Res. Develop. <u>32</u> 127–136 (1988)

for quantum Langevin equations and many other places. Because the formal closure is an exact consequence of the equations of motion, it agrees with systematic, asymptotic closures when those exist.