

Averaging and Coarse-Graining in Systems with Separation of Time-Scales

I. Timofeyev

University of Houston

A. J. Majda and E. Vanden-Eijnden; NYU

Related Publications:
<http://www.math.uh.edu/~ilya>

Outline

- Example 1: Slow Manifold Example
- Example 2: Averaging Example for SDEs
- Connection with Heterogeneous Multiscale Methods (W. E, B. Engquist, E. Vanden-Eijnden, etc.)
- Example 3: Homogenization (Coarse-Graining) Example
- Averaging Derivation
- Homogenization (Coarse-Graining) Derivation
- Derivation for the Triad Example
- WILL ADD SHORTLY: Numerics for the Triad Example

Motivation:

Eliminate the fast degrees of freedom in multiscale systems and derive an effective (stochastic) model for the slow variables. The main objective is to reproduce the statistical properties of the slow variables in full simulations.

Example 1: Deterministic Slow Manifold Approach

Consider:

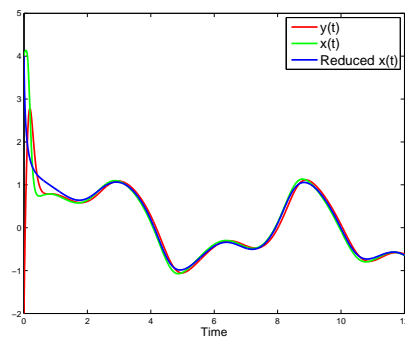
$$\dot{x} = -y^3 + \sin(2t) + \cos(\sqrt{3}t)$$

$$\dot{y} = -\frac{1}{\epsilon}(y - x)$$

Slow Manifold: $y = x$

Reduced Equation:

$$\dot{x} = -x^3 + \sin(2t) + \cos(\sqrt{3}t)$$



Example 2: Averaging in Stochastic Systems (Avective Time-Scale)

Fluctuations of y are important in this case!

Consider System:

$$\begin{aligned}\dot{x} &= -y^3 + \sin(2t) + \cos(\sqrt{3}t) \\ \dot{y} &= -\frac{1}{\varepsilon}(y - x) + \frac{1}{\sqrt{\varepsilon}}\dot{W}\end{aligned}$$

Assume y is much faster; thus we treat x as fixed

Invariant Density for y can be computed explicitly:

$$p(y|x) = \frac{1}{\sqrt{\pi}} e^{-(y-x)^2}$$

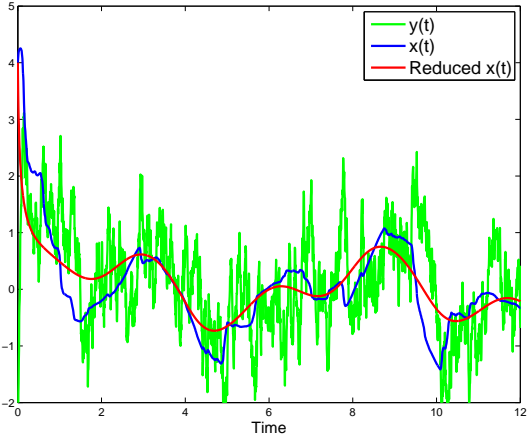
Reduced Equation:

$$\dot{x} = -x^3 - \frac{3}{2}x + \sin(2t) + \cos(\sqrt{3}t)$$

Averaging in Stochastic Systems

Simulations for the example on Averaging:

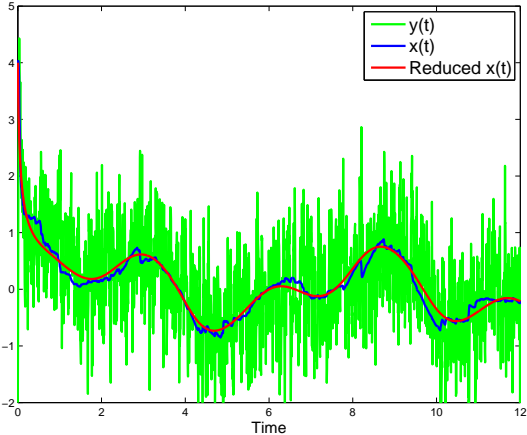
$\varepsilon = 0.1$



Averaging in Stochastic Systems

Simulations for the example on Averaging:

$$\varepsilon = 0.01$$



General Setup for Multi-Scale Systems

Dynamical System : $\dot{Z} = f(Z)$

Decomposition:

$$\begin{aligned} Z &= (SLOW, FAST) \\ &= (Essential, Non - Essential) \end{aligned}$$

Goal: Eliminate Fast modes; Derive Closed-Form equation for Slow Dynamics

Develop Efficient Numerical Algorithms for Fast Integration of Slow Variables

Warning: Slow-Fast Decomposition can be non-trivial; There are many examples with “hidden” slow or fast variables

Asymptotic Approach:

Introduce ε such that

$$\text{Limit } \frac{\text{Time Scale}\{FAST\}}{\text{Time Scale}\{SLOW\}} \rightarrow \infty \text{ as } \varepsilon \rightarrow 0$$

Connection with Heterogeneous Multiscale Methods

Averaging for Stochastic systems is also very closely related to the Heterogeneous Multiscale Methods (W. E, B. Engquist, E. Vanden-Eijnden, etc.)

Stiff Dynamical System (ODE):

$$\begin{aligned}\dot{x} &= g(x, y) \\ \dot{y} &= \frac{1}{\varepsilon} h(x, y)\end{aligned}$$

Q: How to efficiently compute $x(t + \Delta t)$ given $x(t)$?

Nested Procedure:

1. Given $x(t) \equiv \bar{x}$ integrate $\dot{y} = \frac{1}{\varepsilon} h(\bar{x}, y)$ with time step $\delta t \ll \Delta t$ and compute $\langle g(\bar{x}, y) \rangle$; \bar{x} is just a parameter
2. Make “BIG STEP” Δt by integrating $\dot{x} = \langle g(x, y) \rangle$

Example 3: Homogenization (Longer Diffusive Time-Scale)

Consider System:

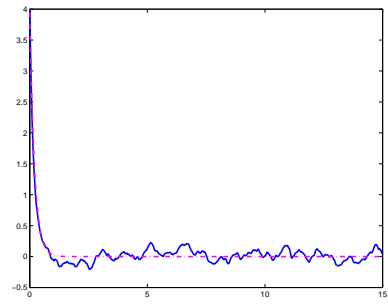
$$\dot{x} = -5x + y, \quad \dot{y} = -10y + \sqrt{10}W$$

Stationary Distribution for y :

$$p(y) = \frac{1}{\sqrt{\pi}} e^{-y^2}$$

Reduced Equation (Averaging FAILS!) Fluctuations are not reproduced by the reduced equation

$$\dot{x} = -5x$$



$x(t)$ with IC $x(0) = 4$

Homogenization - How to FIX the approach

Consider Modified equation:

$$\begin{aligned} \dot{x} &= -\varepsilon 5x + y, \\ \dot{y} &= -\frac{1}{\varepsilon} 10y + \frac{1}{\sqrt{\varepsilon}} \sqrt{10} \dot{W} \end{aligned}$$

Consider Coarse-Grained (Longer) Time

$$\tau = \varepsilon t$$

Rescaled System

$$\dot{x} = -5x + \frac{1}{\varepsilon} y, \quad \dot{y} = -\frac{1}{\varepsilon^2} 10y + \frac{1}{\varepsilon} \sqrt{10} \dot{W}$$

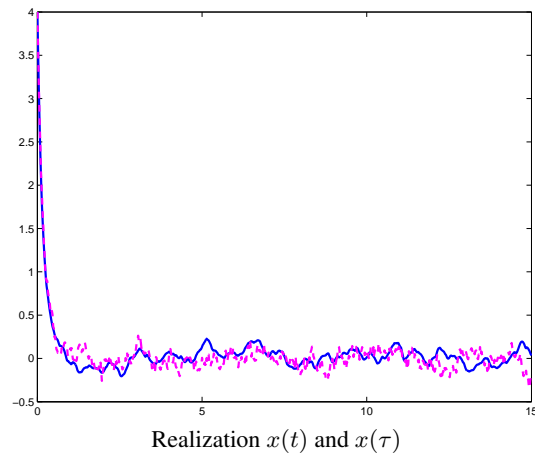
Reduced Equation is a Diffusion:

$$\dot{x} = -5x + (10)^{-1/2} \dot{W}$$

Homogenization: Computational Comparison

Comparison of the Original Full Model and the SDE Reduced Model (Diffusion)

Compare Trajectories:



Note: There is no pathwise convergence, but the fluctuations of $x(t)$ are perfectly reproduced by $x(\tau)$ in statistical sense.

Averaging Derivation

Consider Multiscale SDE

$$\dot{x} = g(x, y) \quad \dot{y} = \frac{1}{\varepsilon} h(x, y) + s(x, y) \frac{1}{\sqrt{\varepsilon}} \dot{W}$$

Corresponding Backward Equation:

$$\partial_t u(x, y, t) = L_1 u(x, y, t) + \frac{1}{\varepsilon} L_2 u(x, y, t)$$

where $u(x, y, t) = \mathbb{E} [\phi(x_t, y_t) | (x_0, y_0) = (x, y)]$, $u(x, y, 0) = \phi(x, y)$. $\phi(x, y)$ is arbitrary.

Operator L_2 corresponds to the fast sub-system (i.e. equation for y in this case)

$$L_2 = h(x, y) \partial_y + \frac{1}{2} s^2(x, y) \partial_y^2$$

Consider Formal Asymptotics:

$$u(x, y, t) = u_0(x, y, t) + \varepsilon u_1(x, y, t) + o(\varepsilon)$$

Substitute and Collect Powers

$$\begin{aligned} L_2 u_0 &= 0 \\ \partial_t u_0 &= L_1 u_0 + L_2 u_1 \end{aligned}$$

First Equation ($L_2 u_0 = 0$) $\Rightarrow u_0 = u_0(x, t)$, i.e. u_0 is only a function of x and t .

Consider Generator L_2 : It corresponds to the auxiliary fast sub-system

$$\dot{y} = h(x, y) + s(x, y)\dot{W}$$

where x plays the role of a FIXED PARAMETER

Assume: Invariant Measure $\mu(y|x)$ Exists, IM Depends on x as a parameter

Introduce Projection Operator:

$$\mathbb{P}\cdot = \int \cdot \mu(y|x) dy$$

Apply \mathbb{P} to the Second equation

$$\mathbb{P}\partial_t u_0 = \mathbb{P}L_1 u_0 + \mathbb{P}L_2 u_1$$

We can use

$$\mathbb{P}L_2 \cdot = 0$$

b/c $\mu(y|x)$ is the density for the auxiliary system (satisfies the FP equation with adjoint the L_2^*)

Also,

$$\mathbb{P}\partial_t u_0 = \partial_t u_0$$

b/c u_0 is a function of only x and t .

We obtain the Reduced Equation:

$$\partial_t u_0 = \mathbb{P}L_1 u_0$$

The above equation is a backward equation for $u_0 \equiv u_0(x, t)$.

This backward equations corresponds to an equation for the variable x :

$$\dot{x} = \int g(x, y) \mu(y|x) dy = \langle g(x, y) \rangle_{\mu(y|x)}$$

Coarse-Graining Derivation
Consider Rescaled Equations

$$\begin{aligned} \dot{x}_t &= -5x_t + \frac{1}{\varepsilon}y_t \\ \dot{y}_t &= -\frac{\gamma}{\varepsilon^2}y_t + \frac{\sigma}{\varepsilon}\dot{W} \end{aligned}$$

We introduced ε in this particular was to emphasize that the y -variables are faster and to make sure that the y -dependent terms in the equation for x do NOT average out to zero.

Backward Equation for $u(x, y, t)$

$$\partial_t u = L_0 u + \frac{1}{\varepsilon} L_1 u + \frac{1}{\varepsilon^2} L_2 u$$

with $L_0 = L_0(x)$, i.e. L_0 includes only self-interactions of slow variables, x

L_2 is the backward operator for the fast sub-system (the right-hand side of x in this case)

Formal Asymptotics

$$u = u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + o(\varepsilon^2)$$

Substitute and Collect Powers

$$L_2 u_0 = 0$$

$$L_2 u_1 = -L_1 u_0$$

$$\partial_t u_0 = L_0 u_0 + L_1 u_1 + L_2 u_2$$

First Equation $\Rightarrow u_0 = u_0(x, t)$
b/c L_2 involves derivatives w.r. to y and u_0 is arbitrary.

Introduce Projection Operator:

$$\mathbb{P} \cdot = \int \cdot \mu(y) dy$$

where $\mu(y)$ is the Invariant Measure of the fast subsystem (the SDE which corresponds to L_2)

Note: The fast sub-system does not have to be identical to the right-hand side of the y -variables; there might be terms in the equation for y which involve ε^{-1} , not ε^{-2} .

Note: $\mathbb{P}L_2 \cdot = 0$ b/c $\mu(y|x)$ is the density for the auxiliary system, i.e. satisfies the FP equation with adjoint the L_2^*

Second Equation Applying \mathbb{P} to the second equation we obtain (Remember: $\mathbb{P}L_2 = 0$)

$$0 = \mathbb{P}L_1 u_0$$

Compatibility Condition: $\mathbb{P}L_1 = 0$

From the Second Equation: $u_1 = -L_2^{-1}L_1 u_0$ (if the compatibility condition holds)

Compatibility Condition pg1

On the previous slide we obtained a compatibility condition

$$\mathbb{P}L_1 = 0.$$

This compatibility condition must hold in order for the homogenization approach to be applicable. The compatibility condition is sometimes written as

$$\mathbb{P}L_1\mathbb{P} = 0$$

to emphasize that $\mathbb{P}L_1$ applied to any function of x must be zero.

The operator L_1 typically involves first-order derivatives w.r. to x and y , i.e.

$$L_1 = A(x, y)\partial_x + B(x, y)\partial_y$$

$B(x, y)\partial_y$ does not matter b/c $\mathbb{P}L_1$ is applied to a function of only x .

Compatibility Condition pg2

$A(x, y)\partial_x$ comes from the ε^{-1} terms of the drift in the equation for x -variables. Therefore, the compatibility condition can be rewritten as

$$\int A(x, y)\mu(y)dy = 0$$

where $A(x, y)$ are the ε^{-1} terms of the drift in the equation for x -variables and $\mu(y)$ is the Invariant Measure of the Fast Sub-System. This is equivalent to AVERAGING=0 condition and must be verified for each system under consideration

Third Equation Apply \mathbb{P} to the third equation

$$\mathbb{P}\partial_t u_0 = \mathbb{P}L_0 u_0 + \mathbb{P}L_1 u_1 + \mathbb{P}L_2 u_2$$

1. $\mathbb{P}L_0 = L_0$ b/c L_0 only depends on x
2. $\mathbb{P}L_2 = 0$
3. Substitute $u_1 = -L_2^{-1}L_1 u_0$

Effective Equation:

$$\partial_t u_0 = L_0 u_0 - \mathbb{P}L_1 L_2^{-1} L_1 u_0$$

Back to our Example:

$$\begin{aligned} \dot{x}_t &= -5x_t + \frac{1}{\varepsilon}y_t \\ \dot{y}_t &= -\frac{\gamma}{\varepsilon^2}y_t + \frac{\sigma}{\varepsilon}\dot{W} \end{aligned}$$

In the Example Above

$$L_1 = y\partial_x$$

L_2 : Generator of the y OU process

$\mu(y)$: Gaussian density

$$\begin{aligned} -\mathbb{P}L_1L_2^{-1}L_1 &= -\int \mu(y)y\partial_xL_2^{-1}y\partial_xdy = \\ -\partial_x^2 \int [yL_2^{-1}y] \mu(y)dy &= -\partial_x^2\mathbb{E}_\mu [yL_2^{-1}y] \end{aligned}$$

where $\mathbb{E}_\mu [yL_2^{-1}y]$ is the expectation w.r. to the stationary distribution of the y -variables in the fast sub-system

We already see that the correction will be a diffusion, but we need to compute the coefficient. We need to understand the action of L_2^{-1} .

Compatibility Condition

The compatibility condition is clearly satisfied for this equation since

$$L_1 = y\partial_x$$

and since $\mu(y)$ is a Gaussian density with mean zero

$$\int y\mu(y)dy = 0$$

Therefore, we can apply the homogenization derivation to this model.

Action of L_2^{-1} :

$$L_2^{-1}f(y) = - \int_0^{\infty} \mathbb{E}[f(Y_t)|Y_0 = y] dt$$

where Y_t is the solution of the fast sub-system at time t and $\mathbb{E}[f(Y_t)|Y_0 = y]$ is the conditional expectation w.r. to Y_t .

The correction becomes

$$-\partial_x^2 \mathbb{E}_\mu [y L_2^{-1} y] = \partial_x^2 \int_0^{\infty} \mathbb{E}_\mu y [\mathbb{E}[Y_t|Y_0 = y]] dt = \partial_x^2 \int_0^{\infty} \mathbb{E}[y Y_t] dt$$

where I switched the order of integrals w.r. to dt and dy , etc. And Y_t is the solution of the fast sub-system with the initial condition $Y_0 = y$.

The object $\mathbb{E}[y Y_t]$ is the stationary correlation function of the fast sub-system.

Reduced Model

For our example, the stationary correlation function of the fast sub-system can be computed explicitly

$$\mathbb{E} [yY_t]_y = \frac{\sigma^2}{2\gamma} e^{-\gamma t}$$

$$\partial_x^2 \int_0^\infty \frac{\sigma^2}{2\gamma} e^{-\gamma t} dt = \partial_x^2 \times \text{Area under the correlation of } y_t = \partial_x^2 \frac{\sigma^2}{2\gamma^2}$$

Generator of the Effective Equation:

$$L = L_0 + \frac{1}{2} \frac{\sigma^2}{\gamma^2} \partial_x^2$$

Effective Equation:

$$dx = -5xdt + \frac{\sigma}{\gamma} dW$$

References

- Khasminsky, R. Z. 1963, 1966
- Kurtz, T. G. 1973, 1975
- Papanicolaou, G. 1976
- Ellis, R. S.; Pinsky, M. A. 1975

MTV <http://www.math.uh.edu/~ilya/papers/>

- Physica D 2002
- JAS 2003
- Nonlinearity 2006
- Physica D 2004
- TCFD 2012

More Complicated Triad Example

The following triad model is a nice example to understand the mode-reduction.

$$\begin{aligned}dx &= A_1 yz dt \\dy &= A_2 xz dt - \gamma y dt + \sigma dW_1 \\dz &= A_3 xy dt - \gamma z dt + \sigma dW_2\end{aligned}$$

with $A_1 + A_2 + A_3 = 0$, so that the energy is conserved by the nonlinear interactions. Also, we assume that γ and σ are pretty large, so that y, z are much faster than x . Therefore, we can introduce ε into the equation to accelerate y and z even more

Accelerated Triad

$$\begin{aligned}dx &= A_1 y z dt \\dy &= A_2 x z dt - \frac{\gamma}{\varepsilon} y dt + \frac{\sigma}{\sqrt{\varepsilon}} dW_1 \\dz &= A_3 x y dt - \frac{\gamma}{\varepsilon} z dt + \frac{\sigma}{\sqrt{\varepsilon}} dW_2\end{aligned}$$

Note: The drift and the diffusion terms are of the same ε^{-1} order in the Fokker-Planck (and backward) equation

Note: The fast sub-system in this case is

$$\begin{aligned}d\tilde{y} &= -\gamma \tilde{y} dt + \sigma dW_1 \\d\tilde{z} &= -\gamma \tilde{z} dt + \sigma dW_2\end{aligned}$$

which is NOT the same as the right-hand side of y and z

The stationary measure of the FAST SUB-SYSTEM is a product measure

$$\mu(\tilde{y}, \tilde{z}) = \frac{2\gamma^2}{\pi\sigma^4} e^{-\frac{\gamma}{\sigma^2} \tilde{y}^2} e^{-\frac{\gamma}{\sigma^2} \tilde{z}^2}$$

Averaging or Homogenization?
Applying Averaging Gives

$$\dot{x} = 0$$

since $\mathbb{E}[yz] = 0$ w.r. to the measure on the previous slide.

We need to coarse-grain time $t = \varepsilon t$

$$\begin{aligned} dx &= \frac{1}{\varepsilon} A_1 yz dt \\ dy &= \frac{1}{\varepsilon} A_2 xz dt - \frac{\gamma}{\varepsilon^2} y dt + \frac{\sigma}{\varepsilon} dW_1 \\ dz &= \frac{1}{\varepsilon} A_3 xy dt - \frac{\gamma}{\varepsilon^2} z dt + \frac{\sigma}{\varepsilon} dW_2 \end{aligned}$$

and apply the homogenization formalism to the rescaled equations above.

Backward Equation for the Triad

$$\partial_t u = \frac{1}{\varepsilon} L_1 u + \frac{1}{\varepsilon^2} L_2$$

Note: $L_0 = 0$ in our previous notation.
Operators L_1 and L_2 are

$$L_1 = A_1 y z \partial_x + A_2 x z \partial_y + A_3 x y \partial_z$$

$$L_2 = -\gamma y \partial_y + \frac{\sigma^2}{2} \partial_y^2 - \gamma z \partial_z + \frac{\sigma^2}{2} \partial_z^2$$

And the effective operator is the same as before

$$L = -\mathbb{P} L_1 L_2^{-1} L_1$$

where \mathbb{P} is the projection operator w.t. to the invariant measure of the fast sub-system

Computing the Effective Operator (pg 1)

Assume the expansion

$$u = u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \dots$$

and, as before, substitute and collect powers of ε . We also obtain that $u_0 = u_0(x, t)$, i.e. does not depend on y -variables
Since the effective operator L will be applied to $u_0 = u_0(x, t)$ we can neglect ∂_y and ∂_z on the right, i.e.

$$L = -\mathbb{P}L_1L_2^{-1}L_1u_0 = -\mathbb{P}L_1L_2^{-1}A_1yz\partial_x$$

We have to be careful with ∂_x since L_1 involves x ; Cannot pull ∂_x through the integral
Therefore, we have to compute

$$\mathbb{P}[A_1yz\partial_x + A_2xz\partial_y + A_3xy\partial_z]L_2^{-1}A_1yz\partial_x$$

Computing the Effective Operator (pg 2)

We have to compute

$$\mathbb{P}[A_1yz\partial_x + A_2xz\partial_y + A_3xy\partial_z]L_2^{-1}A_1yz\partial_x =$$

$$\mathbb{P}A_1yz\partial_xL_2^{-1}A_1yz\partial_x + \mathbb{P}[A_2xz\partial_y + A_3xy\partial_z]L_2^{-1}A_1yz\partial_x =$$

Part 1 + Part 2

We will compute these two parts separately.

Computing the Effective Operator (pg 3)

First Part: (we can pull ∂_x outside b/c L_2 does not depend on x)

$$-\mathbb{P}A_1yz\partial_x L_2^{-1}A_1yz\partial_x = A_1^2\partial_x^2 \int_0^\infty \langle yzy_tz_t \rangle_\mu dt = A_1^2 \left(\frac{\sigma^2}{2\gamma} \right)^2 \frac{1}{2\gamma} \partial_x^2$$

$$\langle yzy_tz_t \rangle_\mu = \langle yy_t \rangle_\mu \times \langle zz_t \rangle_\mu = \left(\frac{\sigma^2}{2\gamma} \right)^2 e^{-2\gamma t}$$

Second Part: (we need to be careful b/c L_1 involves ∂_y and ∂_z)

$$-\mathbb{P}A_2xz\partial_y L_2^{-1}A_1yz\partial_x = A_2A_1x\partial_x \mathbb{P} \frac{y}{v^2} z L_2^{-1}yz =$$

$$A_2A_1x\partial_x \frac{1}{v^2} \int_0^\infty \langle yzy_tz_t \rangle_\mu dt = A_2A_1x\partial_x \frac{v^2}{2\gamma}$$

where $v^2 = \sigma^2/(2\gamma)$ and we we integrated by parts and shifted ∂_y onto $\mu(y, z)$

Similarly:

$$-\mathbb{P}A_3xy\partial_z L_2^{-1}A_1yz\partial_x = A_3A_1x\partial_x \frac{v^2}{2\gamma}$$

Computing the Effective Operator (pg 4)

Second Part Together: (use $A_1 + A_2 + A_3 = 0$)

$$-\mathbb{P}[A_2xz\partial_y + A_3xy\partial_z]L_2^{-1}A_1yz\partial_x = -A_1^2\frac{1}{\sigma^2}\left(\frac{\sigma^2}{2\gamma}\right)^2x\partial_x$$

Effective Generator:

$$L = -gx\partial_x + \frac{s^2}{2}\partial_x^2$$

Effective Equation:

$$dx = -gxdt + sdW$$

where

$$g = A_1^2\frac{\sigma^2}{4\gamma^2}, \quad s = A_1\frac{\sigma^2}{2\gamma\sqrt{\gamma}}$$