

Lightening the Performance Burden of Individual-Based Models through Dimensional Analysis and Scale Modeling

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1 Introduction

Systems models of larger populations (such as those used for health policy, ecological studies, marketing, urban planning, etc.) have traditionally tended to be aggregate, in the sense that a particular state variable summarizes information on many individuals. Such aggregate models offer many virtues, including greater transparency, ease of analysis and calibration. However, modeling considerations sometimes motivate the use of finer-grained models. Such factors include the need to evaluate interventions targeted at an individual level particular individuals (e.g. such as are increasingly used in infectious disease epidemiology), to understand transfer effects or dynamic impacts of heterogeneity on intervention effectiveness, the dynamics of complex and adaptive network structures, and memoryful transition processes. Such concerns have fostered the popularity of individual-based models, which explicitly describe and simulate the attributes and behavior of each member of a population. Behavior within such individual-based models can be formulated in many different ways, including using classic state-equation methods (using ordinary differential equations) or with discrete objects and rules (as is typical in classic agent-based modeling).

While individual-based approaches offer considerable value for addressing certain types of questions and problems, such models impose higher (and frequently dramatically higher) performance costs. The heavy performance burden associated with large-scale individual-based models reflects several factors. The first is the simple cost of updating a state vector of size proportional to the count of individuals in the population (which we term n). Even a model where each individual evolves completely independent of others will experience linear performance scaling; for large populations and significant amounts of individual state this can impose a very heavy burden (not least because of memory hierarchy effects). Models with highly connected populations will often exhibit performance costs that rise superlinearly with population size. For example, a model in which each individual is connected to a small fraction α of other individuals in the population will impose performance costs that rise at least proportional to n^2 (i.e. $\Omega(n^2)$). Thirdly, because individual behavior and dynamics (e.g. infection spread from one individual to another, or the decision of an individual to cease smoking) often involves some stochastic factors, individual-based models often require consideration of stochastic processes. Gaining an appreciation for the behavior of a given fully parameterized model often requires evaluation of a Monte Carlo ensemble of realizations – a process that can require a day or more of simulation time.

In addition to inhibiting exploratory learning and user involvement, prolonged model simulation times can also impose significant opportunity costs that can reduce the value delivered by the model. For example, long simulation times can rule out interactive model exploration and considerably reduce the amount of focused model exploration that is possible – thereby impeding a modeler’s understanding of a model’s dynamics. The longer cycle time associated with understanding each version of the model performance burden can also reduce the opportunities for model refinement.

In light of the above performance concerns, creators of individual-based models involving large populations are often tempted to draw insights from simulations involving subsamples of the full population [1]. Unfortunately, while working with subpopulations can greatly lessen performance burdens, it can also be deceiving: Naïve intuition may mislead one into believing that reduction of a population size by some factor should be

accompanied by a similar reduction in all parameters – a transformation that may qualitatively alter the behavior of the model and make results of the reduced-scale model completely unrepresentative of the full-scale model. Even given an adequate reduced-scale model, it is often unclear how to scale up results from a reduced-scale model to correspond the results that would obtain for a full population. Indeed, as we will see, this scaling can be quite complex, involving power laws and ratios of other parameters.

Drawing inspiration from the widespread and critical role that *dimensional analysis and scaling* have played in engineering and the physical sciences, this paper proposes the use of these tools to address the performance challenges associated with individual-based models. Specifically, we propose a precise, rigorous, systematic and general-purpose technique to formulating reduced-scale individual-based models. Measurements of output parameters of such reduced-scale models can then be precisely transformed (in accordance with model scaling laws) to yield comparable results for a full-scale model – without the need to run the full-scale model. It is notable that these techniques are notable in relying only upon dimensional homogeneity of the full-scale model, and on not the specifics of model behavior or use of a particular mathematical framework.

The remainder of the paper is organized as follows. The next section of this paper explains some basic concepts of dimensional analysis. A key component of this section is the recognition that any real-world system – or any dimensionally homogeneous model [2] – must be amenable to description in a fashion that is independent of unit systems – a model, therefore, which involves only *dimensionless variables*. The following section introduces the notion of *similitude*, which provides the basis for scale models. The next section simultaneously describes and illustrates (with an example) a systematic means for deriving scale models from full-sized models with precisely specified parameter values. The final section of the paper provides a brief summary of the paper and lays out prospects for additional work.

2 Dimensional Analysis

Dimensional analysis rests upon the concept of dimensional quantities. Physical quantities can be associated with semantic categories (the ‘Dimension’ of the quantity, such as “Person”, “Time”, “Length³”, “Liquid Volume”), as well as the standard of reference for measuring/sizing the quantity (the ‘Units’ of the quantity, such as “Day”, “cubic foot”, “gallon”) [3, 4].

Dimensional quantities are associated with a formal dimensional algebra that differs in important ways from the algebras on non-dimensional quantities, such as real numbers [5]. Within such an algebra, we associate each dimensional quantity with a product of powers of different units (or dimensions), i.e. $d_1^{i_1} d_2^{i_2} d_3^{i_3} \dots d_n^{i_n}$, where there exist exactly n dimensions of concern to us, where each exponent i_j represents the power to which the corresponding dimension d is included, and where the ordering of the dimensions d is arbitrary. For example, *Mortality* might be associated with units Person¹/Day i.e. Person¹*Day⁻¹ (and of dimension Person¹*Time⁻¹). A notable class of quantities is those associated with *unit* dimension (commonly called *dimensionless*¹, although this is somewhat of a misnomer) – i.e. where $i_1=i_2=\dots=i_n=0$.

The dimensions associated with a given quantity (in this case Person¹*Time⁻¹) can be used in a straightforward fashion to indicate how the value of a given quantity would change given a change in unit systems. For example, if we were to change our chosen measurement for people from individual persons to thousands of people (a factor of 1000 increase) it follows that the numerical value of a quantity whose dimension of Person¹*Time⁻¹ would be divided by value 1000¹. Similarly, if we were to change the measurement for time from days to weeks (a factor of 7 increase), the numeric value of the resulting quantity would be divided by 7⁻¹ (i.e. multiplied by 7). Given a

¹ Strictly speaking, the term “dimensionless” is a misnomer. While “Dimensionless” quantities have no dependence on the units by which we measure any dimension, such quantities are no more dimensionless than quantities of 0 length are “lengthless”. “Dimensionless” quantities have a dimension, just a very special dimension – one in which the exponent of every dimension is identically 0. A better (or at least less abusive) name is “unit” dimension. Nonetheless, we cede to convention in using the term “dimensionless” in this document.

dimensioned quantity whose dimensions include the term d^i , increasing the magnitude of the unit of measurement of a dimension d by a factor of x will lead the numeric value of that quantity to be divided by a factor of x^i . “Dimensionless” quantities are particularly notable in that their numeric values are *independent* of the units system employed – that is, they retain their values regardless of our measurement conventions. As will be discussed below, such quantities play a critical role in real-world systems.

Mathematical operators can be extended to dimensional quantities in consistent manners [5]. For example, multiplication of quantities drawn from two different unit (dimension) systems yields a product with units (dimensions) that are composed of a product of powers of each unit (dimension), where the exponent on a given unit is just the sum of the exponents on that unit (dimensions) (possibly zero) for each of the quantities being multiplied. In general, the presence of dimensional quantities aids the modeling process by imposing additional structure that significantly constrains the set of legitimate formulations that can be considered in a given problem. For example, addition of dimensional quantities are not defined unless both quantities possess identical units² and dimensions. It follows from these results that a dimensioned quantity in an (for example) exponent or trigonometric function must be of unit dimension. Matrix algebra, state equations, and other mathematical constructs have been systematically extended to dimensioned quantities [5].

By far the most common use of dimensional analysis – and one widespread within the Systems Dynamics community – is as a simple check the correctness of formulas. While dimensional analysis delivers considerable value in this capacity, the ideas are vastly deeper than is commonly realized, and the full value of the approach extends far beyond dimensional bookkeeping on exponents [6].

3 Similitude

3.1 The Buckingham Pi Theorem

3.1.1 Background

This section focuses on the notion of *similitude*, which provides the basis for scale models. We first introduce the Buckingham³ Pi Theorem [7, 8], which states that any dimensionally consistent model of a physical system can be formulated in a fashion that involves only dimensionless parameters. Because dimensionless parameters are invariant to unit change, such a representation is independent of measurement system. It follows that that two instances of a systems model having different population sizes and having identical values for all dimensionless parameters must exhibit “similar” behavior⁴. We then discuss a systematic approach for identifying the dimensionless variables associated with a model and determining an exact relationship relating the scaling of a given *dependent* variable in terms of other model governing parameters. Finally, we describe a procedure that, given a complete specification for the parameters values of a full-scale model, permits us to derive the parameters of a reduced-scale model offering desirable values for particular parameter values (such as the population size).

We begin this section by adopting the widely held assumption that the processes of the real world operate regardless of which measurement systems we use to describe those processes. On the basis of this assumption, we can say with confidence that whatever equations govern (and describe) those real-world processes, they must operate independent of unit systems.

² Addition of quantities drawn from separate unit system but the same dimensions cannot be performed unless the quantities are scaled by the appropriate unit conversions. It is simply nonsensical to add quantities drawn from different dimensions.

³ Note that although the Theorem carries Buckingham’s name, there is good reason to think that the critical ideas originated decades earlier.

⁴ We ignore here discretization effects, which play an important role for smaller models.

At the most basic level, the Buckingham Pi Theorem [7] builds upon two key observations: This invariance of real-world systems to unit systems, and the fact that only dimensionless quantities are independent of unit systems. Informally, the Pi Theorem states that one can respecify any legitimate dimensionally homogeneous equation using an equation involving only dimensionless quantities.

More specifically, consider a dimensionally consistent (homogeneous) equation relating n dimensional quantities (*governing parameters*) $x_1 \dots x_n$ and associated with r independent⁵ dimensional products. Without loss of generality, assume that x_1 is the dependent variable:

$$x_1 = f(x_2, x_3, x_4, \dots, x_n)$$

This equation can always be reformulated as an equation involving only $(n-r)$ *dimensionless parameters* Π_i .

$$\pi_1 = \Psi(\pi_2, \pi_3, \pi_4, \dots, \pi_{n-r})$$

Each of these dimensionless parameters π_i is defined as a product of powers of the original governing parameters $x_1 \dots x_n$ such that the exponents of each dimension balance to 0 and their product is dimensionless. π_1 is the unique *dependent* dimensionless parameter, and is the sole dimensionless parameter involving the dependent variable x_1 . Given that π_1 is defined as a product of powers of the x_i , the relationship between x_j and π_1 is such that:

$$\pi_1 \equiv \frac{x_1^{d_1}}{\prod_{i=2}^k x_i^{d_i}}$$

Where $0 \leq k \leq n-d$ is the number of other governing parameters x_i needed to multiply (divide) x_j in order to make the product dimensionless.

Moreover, a deeper result of the Pi Theorem indicates that *any* dimensionally consistent (homogeneous) model can be reformulated in this fashion. It bears stressing that while the above equations appear algebraic, the Buckingham Pi Theorem holds for equations in general – including Ordinary, Stochastic and Partial Differential Equations.

3.1.2 Advantages of the Π Theorem

While it may initially appear a mere curiosity, The Buckingham Pi Theorem has a number of significant implications. While the Buckingham Pi Theorem describes a deep fact about relations between dimensional quantities in the real world, we can take advantage of our knowledge of this theorem when we specify models of the external world. Specifically, secure in the knowledge that relations between quantities in the world can be described using only dimensionless quantities, we can confine our attention to building models of the real world that use only dimensionless parameters (π_i).

Explicitly working with models involving only dimensionless parameters offers a number of significant advantages. Firstly, consider the amount of effort needed to statistically estimate a mathematical model relating of n governing parameters (in d independent dimensions), as compared to the corresponding mathematical model involving only $(n-d)$ dimensionless quantities. Because of the curse of dimensionality, the dimensionless mathematical model will often require orders of magnitude fewer parameters to estimate than would the naïve statistical model [9]. Secondly, formulating from the start a model involving only dimensionless variables allows us to transparently switch between different unit systems, without any change to the model.

⁵ We refer to independence in a linear algebraic sense, where the vector space has axes for each dimension of concern, and each vector uniquely represents a unique product of dimensions. The value of the vector along a particular dimension is given by the exponent associated with that product of dimensions.

Thirdly, the identification of the dimensionless parameters and knowledge that they are linked through some (typically unknown) function Ψ can provide insight into how a system must function. The dimensionless parameters being used by such a model (e.g. the Reynolds Numbers, Fourier Number, Raleigh Number, Mach Number) frequently have deep and recurring physical significance. Conceptualizing the world in terms of such dimensionless quantities can provide insight into causal regularities, and particularly into scaling properties and invariants. The level of insight gained through the Buckingham Pi Theorem does vary between problems; the insights gained from models employing few dimensionless parameters can be particularly striking. Insights can be sharpened by a variety of techniques, including refinement of the dimensional system via dimension splitting [8], fusion of tightly coupled governing parameters [8], and reasoning based on intermediate asymptotics [9, 12].

3.2 Similar Systems

Consider two real-world systems A and B associated with the same set of governing parameters x_i pertinent to the phenomenon of interest, where those parameters are governed by the same fundamental processes. Although A and B share identical sets of governing parameters, the two systems may differ with respect to the particular value of these governing parameters. For example, A could be a full-size aircraft, and B a reduced-size aircraft for wind-tunnel experiments. Alternatively, A may be a large antenna, and B electrical engineer's small-scale model thereof, or perhaps A is a bridge, and B a smaller replica of that bridge for structural testing. For our purposes, A could be a full-scale simulation model and B a reduced-scale model. Call the particular values associated with those governing parameters in systems A and B $x_{i,FS}$ and $x_{i,RS}$. (Note that while we adopt subscriptions suggestive of "full-scale" and "reduced-scale" for the sake of clarity in later discussion involving reduced-scale models, the notion of dimensional similarity by no means requires that either A or B is a systematically reduced version of the other. Indeed, in comparison to A's governing parameters, B's governing parameters may be larger, smaller, or some combination thereof.)

Following the previous section, such systems have a (frequently unknown) relation giving dependent variable x^A_i (or x^B_i) as a function of the other governing parameters. Thus

$$x_{1,FS} = f(x_{2,FS}, x_{3,FS}, x_{4,FS}, \dots, x_{n,FS})$$

and

$$x_{1,RS} = f(x_{2,RS}, x_{3,RS}, x_{4,RS}, \dots, x_{n,RS})$$

It bears emphasizing that because we assume that A and B are governed by the same processes, f is the same function in both cases.

We know from the Buckingham Pi Theorem that these equations can be rewritten in the form

$$\pi_{1,FS} = \Psi(\pi_{2,FS}, \pi_{3,FS}, \pi_{4,FS}, \dots, \pi_{n-r,FS})$$

and

$$\pi_{1,RS} = \Psi(\pi_{2,RS}, \pi_{3,RS}, \pi_{4,RS}, \dots, \pi_{n-r,RS})$$

We term A and B *similar* if $\forall i, 1 \leq i \leq n, (\pi_{i,FS} = \pi_{i,RS})$. That is, two systems that may be very different in terms of the particular values of their parameter sets $x_{i,FS}$ and $x_{i,RS}$ are considered similar if all dimensionless variables share the same values in each of these two systems. The notion of *dimensionally similar* is important in that the Buckingham Pi Theorem reveals that two similar systems are really "the same system," the difference between them being one merely of scale. Thus we can think of a model reformulated so as to use only dimensionless parameters as defining equivalence classes of systems. Each member of these equivalence classes

shares with all others in the same equivalence class identical values for all dimensionless parameters in the (reformulated) system.

We note that because $\pi_{1,FS}$ is purely a function of the other $\pi_{i,FS}$ (and similarly for $\pi_{1,RS}$) and because the relation Ψ is identical for both A and B, A and B are similar if

$$\forall i, 2 \leq i \leq n, (\pi_{i,FS} = \pi_{i,RS})$$

From which it must follow that the dependent variables must hold identical values, that is, that $\pi_{1,FS} = \pi_{1,RS}$.

For many decades, scientists and engineers have exploited the concepts of *similarity* to build *dimensionally similar scale models* that behave identical to a full-scale system with respect to clearly-defined class of measures. We now turn to apply this notion to the particular case of individual-based simulations. The next section briefly explains how such scale models are constructed.

3.3 Building Scale Models

Scale modeling is traditionally used to facilitate convenient experimentation with systems in the external world, whether of natural or artificial origin. Reduced-scale models of bridges, buildings, ocean waves, and vehicles are far cheaper and more tractable to work with than are their full-sized counterparts. In most such cases, the relation between the relevant governing parameters is not fully known, but this poses no barrier: Such scale modeling does not any knowledge of the underlying equations, and exploits only the invariance of the behavior of the external world with respect to unit system choice.

Within this paper, we exploit the same basic idea, but with a slightly different twist. While perhaps all previous scale models have focused on real-world artifacts, our modeling target is itself another model— an individual-based simulation model. While traditional scale modeling relies upon the dimensional consistency (homogeneity) of relations between real-world processes, we rely here upon the dimensional consistency of the individual-based simulation model. The dimensional consistency of this model assures us that the Buckingham Pi Theorem applies for any relation relating a dependent governing parameter x_1 to the other the governing parameters of the model $x_2 \dots x_n$. While we need not explicitly derive the corresponding relation involving only dimensionless quantities Π_i , the Pi Theorem guarantees that this relation does exist and provides the basis for subsequent scale modeling.

As an alternative to simulating the full-scale system to measure on a large-scale individual-based model x_1 , we can thus make use instead of a reduced-scale model (one with, for example, a much smaller population) by following the steps below. In order to illustrate these steps, we introduce an ongoing example.

3.3.1 Step 1: Identify Governing Parameters and their Dimensions

Consider an individual-based model of the spread of a zoonotic infectious disease [10, 11]. For such diseases (which include important tropical diseases such as Schistosomiasis, Malaria, and Dengue fever), all secondary infections of a person (Host) occur from an animal (Vector; Snails for Schistosomiasis and Mosquitoes for Malaria and Dengue fever). The etiology of such diseases can be complex, and perhaps our individual-based simulation model includes detailed characterization of immune system response (as affects egg shedding in Schistosomiasis), heterogeneity in disease response (notable for Schistosomiasis), and behavioral factors (as might affect likelihood of exposure to a Vector or the successful transmission of the disease to vectors).

Suppose that we would ideally like to simulate a full-scale individual-based model⁶ having governing parameter values⁷ as follows:

⁶ While we would typically approach the scale-model identification with a specific model in hand, we purposefully omit specification of the equations of such a model for the sake of brevity and communicating the generality of this approach – particularly, the fact that it does not rely on any detail of model specification (except for its dimensional homogeneity).

Description	Parameter	Dimension
Death rates for infected Vectors	μ_v	1/Time
Death rates for infected Hosts	μ_h	1/Time
Per-Contact likelihood of Transmission from hosts to vector	β_v	1 (“Dimensionless”)
Per-Contact likelihood of Transmission from vectors to host	β_h	1
Net migration rate for vectors	M_v	Vector / Time
Net migration rate for hosts	M_h	Host / Time
Recovery rate for infected hosts	α	1/Time
Initial infected hosts	I_{h0}	Hosts
Initial infected vectors	I_{v0}	Vectors
Contact rate	c	Host/(Vector*Time)
Population size for vectors	P_v	Vector
Population size for hosts	P_h	Host
Current time	t	Time

Suppose further that the full-scale model using these parameters imposes an infeasibly high performance burden due to high population sizes of vectors and hosts. We therefore wish to create a reduced-size model (specifically including smaller populations for vectors and hosts) whose outputs we can extrapolate to the full-scale model. While this goal seems obvious enough, it is not immediately clear how reducing the size of the populations should impact the various parameter values. For example, if we were to reduce the population of vectors and hosts by some uniform factor ε , should we reduce the contact rate by the same factor? What of the transmission probabilities? Would the reduced-scale model that is yielded have a timescale equivalent to that of the full-scale model, such that we could apply times read off from the reduced-scale model (e.g. time of maximum prevalence) directly in the context of the full scale model?

3.3.2 Step 2: Identify Dependent Variable

Suppose that we wish to calculate a dependent parameter λ of dimension 1/Time – such as would be associated with a frequency (e.g. frequency of oscillation), a fractional rate of growth, an eigenvalue of the linearized system, etc. Because all of these have identical dimension, they can all be calculated using an identical reduced-scale model and scaling procedure. (As we will see, dependent variables of different dimension can typically be calculated using an identical reduced-scale model, but will require different scaling formulas to extrapolate from the results of the reduced-scale model to those of the full-scale model.)

⁷ Note that some of these parameters are sizes of collections, as in the size of the host and vector population. We adopt much of our notation from a compartment model of the same phenomenon included in the cited references.

3.3.3 Step 3: Identify Expressions for Dimensionless Variables

3.3.3.1 Basics

Recalling the notion of similarity from Section 3.3, we know that any scale model must preserve the value of all independent dimensionless parameters π_i . Two models with identical values for corresponding dimensionless parameters must yield an identical value for the dependent variable no matter how complex Ψ may be. We thus proceed to determine a set of governing parameters for the reduced-scale model (for example, α_{RS} and $M_{h,RS}$) that are both computationally feasible and leave the dimensionless variables for that reduced-scale model ($\pi_{i,RS}$) equal in value to the corresponding $\pi_{i,FS}$.

The first step in this direction is to identify expressions for a set of dimensionless variables Π_i in terms of the dependent variable and plausible governing parameters. This set need not be unique and is straightforward (and nearly mechanical) to derive, being identified through reference to a *dimensional matrix* populated through reflection on the dimensionality of governing parameters and a bit of linear algebra.

For our case dimensional matrix can be defined as follows; the Appendix describes a systematic means by which this and similar matrices can be derived.

	λ	M_h	M_v	μ_h	μ_v	α	I_{h0}	I_{v0}	β_h	β_v	c	P_h	P_v	t
Host	1	1	0	0	0	0	1	0	0	0	1	1	0	0
Vector	0	0	1	0	0	0	0	1	0	0	-1	0	1	0
Time	-1	-1	-1	-1	-1	-1	0	0	0	0	-1	0	0	1
π_1	1	0	0	0	0	0	0	0	0	0	0	-1	0	1
π_2	0	1	0	0	0	0	0	0	0	0	0	-1	0	1
π_3	0	0	1	0	0	0	0	0	0	0	0	0	-1	1
π_4	0	0	0	1	0	0	0	0	0	0	0	0	0	1
π_5	0	0	0	0	1	0	0	0	0	0	0	0	0	1
π_6	0	0	0	0	0	1	0	0	0	0	0	0	0	1
π_7	0	0	0	0	0	0	1	0	0	0	0	-1	0	0
π_8	0	0	0	0	0	0	0	1	0	0	0	0	-1	0
π_9	0	0	0	0	0	0	0	0	1	0	0	0	0	0
π_{10}	0	0	0	0	0	0	0	0	0	1	0	0	0	0
π_{11}	0	0	0	0	0	0	0	0	0	0	1	-1	1	1

Table 1 Example Dimensional Matrix. Shaded portions are specific to the dimensionality of the dependent variable chosen (1/Time).

The first column and 4th row of Table 1 (shaded for reference) are specific to dimensionality (Host/Time) of the dependent variable (λ) we have chosen; the remainder of the table is invariant of the choice of dependent variable.

We can read off the definition of each dimensionless parameter Π_i from the corresponding lower 11 rows of Table 1. Each entry in such rows describes the exponent of the associated governing parameter (as specified by the column) within the dimensionless parameter (as specified by the row).

For our case, the dimensionless parameters are defined as follows:

$$\pi_1 = \frac{\lambda t}{P_h}$$

$$\pi_2 = \frac{M_h t}{P_h}$$

$$\pi_3 = \frac{M_v t}{P_v}$$

$$\pi_4 = \mu_h t$$

$$\pi_5 = \mu_v t$$

$$\pi_6 = \alpha t$$

$$\pi_7 = \frac{I_{h0}}{P_h}$$

$$\pi_8 = \frac{I_{v0}}{P_v}$$

$$\pi_9 = \beta_h$$

$$\pi_{10} = \beta_v$$

$$\pi_{11} = \frac{cP_v t}{P_h}$$

3.3.4 Step 4: Identify Values of Dimensionless Parameters in Full-Scale Model

The next step in deriving a reduced-scale model is to derive the value that each non-dependent dimensionless parameter $\pi_i, i > I$ must hold in the reduced-scale model. We do so based on the known values of the non-dependent governing parameters $x_{i,FS}, i > I$ within the full-scale model. To maintain similar results, we must design the reduced-scale model to maintain identical values all of the dimensionless parameters.

For example, for π_2 we compute as follows:

$$\pi_2 = \frac{M_{h,FS} t_{FS}}{P_{h,FS}}$$

Similar calculations are performed for the other dimensionless parameters, except for the dependent dimensionless parameter π_1 . The latter is to be determined through calculations on the results of empirical measurement.

3.3.5 Step 5: Derive Governing Parameters for the Reduced-Scale Model

In the final step needed to complete the specification of the reduced-scale model, we derive the governing parameters $x_{i,RS}, i > I$ for a reduced-scale system such that all of the non-dependent dimensionless parameters $\pi_i, i > I$ in the reduced-scale model share the same values as their corresponding parameters in the full-scale model.

The derivation of these governing parameters will vary with respect to their position in the dimensional matrix above (see Appendix). The governing parameters in the last several columns of the matrix depicted in Table 1 (those in submatrix C, as defined in the Appendix) are *free parameters* that can be assigned convenient values by the modeler. By contrast, the other governing parameters for the reduced-scale model system are bound parameters to be derived from the free parameters and the corresponding values of the governing parameters in the full-scale model.

The next two subsections describe these parameters for our example.

3.3.5.1 Free Governing Parameters

The free (independent) governing parameters (the quantities associated with the last r columns the dimensional matrix (where r is the count of independent dimensions) are for us to choose. In this model, we assume that the computational expense arises predominantly from the need to simulate the transmission of infection in the (individually represented) populations of vectors and hosts. Suppose that to construct the reduced-scale model we wish to downsample the population by a coefficient of $\varepsilon \ll 1$; thus we wish to have

$$\begin{aligned} P_{h,RS} &= \varepsilon P_{h,FS} \\ P_{v,RS} &= \varepsilon P_{v,FS} \end{aligned}$$

For the final free governing parameter – time t – suppose that we wish to preserve identical timing for the reduced-scale model as that which obtains in the full-size model, thus

$$t_{RS} = t_{FS}$$

3.3.5.2 Bound Governing Parameters

Having determined the free governing parameters of the reduced scale model, we must determine the values of the bound governing parameters in the reduced scale model. While we can perform this process in a fully automated fashion using matrix manipulations (Gaussian Elimination) of the logarithms of coefficients of governing parameters, this section illustrates the process through manual calculations. The Appendix illustrates how similar results can be obtained through inspection.

From the equivalence of dimensionless parameters in the full and reduced-size models, we know that the governing parameters that happen to be dimensionless must hold identical values in the two models, thus:

$$\begin{aligned} \pi_{9,RS} = \pi_{9,FS} &\Rightarrow \beta_{h,RS} = \beta_{h,FS} \\ \pi_{10,RS} = \pi_{10,FS} &\Rightarrow \beta_{v,RS} = \beta_{v,FS} \end{aligned}$$

For other dimensionless variable, the situation is more complex, because they involve multiple governing parameters. For example, consider π_2 :

$$\pi_2 = \frac{M_h t}{P_h}$$

Because we know that $\pi_{2,RS} = \pi_{2,FS}$ it must be the case that

$$\frac{M_{h,RS}t_{RS}}{P_{h,RS}} = \frac{M_{h,FS}t_{FS}}{P_{h,FS}}$$

Recall that

$$P_{h,RS} = \varepsilon P_{h,FS}$$

$$t_{RS} = t_{FS}$$

We can now solve for the size of governing parameter M_h in the reduced-scale model, by simple algebra on the equality above:

$$\frac{M_{h,RS}t_{FS}}{(\varepsilon P_{h,FS})} = \frac{M_{h,FS}t_{FS}}{P_{h,FS}}, \text{ implying that } M_{h,RS} = \varepsilon M_{h,FS}.$$

By following a similar procedure, we recognize that

$$\pi_3 = \frac{M_v t}{P_v} \Rightarrow M_{v,RS} = \varepsilon M_{v,FS}$$

$$\pi_4 = \mu_h t \Rightarrow \mu_{h,RS} = \mu_{h,FS}$$

$$\pi_5 = \mu_v t \Rightarrow \mu_{v,RS} = \mu_{v,FS}$$

$$\pi_6 = \alpha t \Rightarrow \alpha_{RS} = \alpha_{FS}$$

$$\pi_7 = \frac{I_{h0}}{P_h} \Rightarrow I_{h0,RS} = \varepsilon I_{h0,FS}$$

$$\pi_8 = \frac{I_{v0}}{P_v} \Rightarrow I_{v0,RS} = \varepsilon I_{v0,FS}$$

$$\pi_{11} = \frac{cP_v t}{P_h} \Rightarrow c_{RS} = c_{FS}$$

A rapid and methodical approach to deriving such formulas is given in Appendix 2.

3.3.5.3 Parameters of the Reduced-Scale Model: Summary

We have now derived the values of the governing parameters of the reduced-scale model. A few of these (the free governing parameters) were chosen so as to be computationally tractable and convenient, while (bound) governing parameters of the reduced-scale model were specified in terms of a coefficients times the corresponding parameter in the full-scale model – with the value of that coefficient chosen that the values of each dimensionless parameters is equal between the two models.

	λ	M_h	M_v	μ_h	μ_v	α	ρ_v	ρ_h	β_h	β_v	c	t	P_h	P_v
Host	ε	ε	ε	1	1	1	1	1	1	1	1	1	ε	ε

Table 2: Scaling Coefficients for Coupled Infection-Health Services Model. An entry in this table describes the coefficient by which a governing parameter in the reduced-scale model has been multiplied (in comparison to the corresponding governing parameter in the full-scale model).

The results of this investigation are shown the table above. Note that the shaded scaling coefficients were explicitly chosen, while the values of the others were derived by exploiting the equivalence of the dimensionless parameters in the two models.

3.3.6 Step 6: Measure Dependent Governing Parameter from the Reduced Scale Model

The next step in our analysis would be to parameterize the reduced scale model (using the scaling relationships specified in Table 2). The reduced-scale model would then be run and a value for λ_{RS} measured.

3.3.7 Step 7: Calculate Dependent Variable for the Full-Scale Model

The dimensionless parameter π_1 is distinguished from other dimensionless parameters in that π_1 is to be calculated from the measured *output* of the reduced-scale model. From a measured value for the dependent governing parameter of the reduced-scale model (here λ_{RS}), we seek to extrapolate the value of the dependent variable for the full-size model (here λ_{FS}).

Much as Step 5 (Section 3.3.5) calculated the values for bound governing parameters in the reduced-scale model in terms of known scaling coefficients and governing parameter values for the full-scale model, here we use the same process in reverse: We use the this measured value λ_{RS} from the reduced-scale model to calculated λ_{FS} for the full-scale model.

For our example, by the process described in Step 5, we note that the definition $\pi_1 = \frac{\lambda t}{P_h}$ and the fact that

$\pi_{1,RS} = \pi_{1,FS}$ implies that

$$\frac{\lambda_{FS}}{\lambda_{RS}} = \frac{1}{1 \cdot \varepsilon} = \frac{1}{\varepsilon},$$

and thus that

$$\lambda_{FS} = \frac{\lambda_{RS}}{\varepsilon}$$

We have now derived the desired quantity – the dependent variable for the full-scale model – in terms of known quantities – the measured dependent variable of the reduced-scale model and a known (free governing parameter) scaling coefficient. We have been able to deduce the value to be output by the full-scale model without bearing the high cost of simulating the model with the full population.

As noted above, these results would change only slightly based on the dimensionality of the dependent variable. For example, if the dependent variable were of dimension 1/Time (rather than Host/Time), the dimensionless variables would be identical as to the previous case, with the exception of π_1 , which would then be given by the expression

$$\pi_{1,Alternative} = \lambda t$$

and we would have $\lambda_{FS} = \lambda_{RS}$

In general, we can change the dimension of the dependent variable without any need to change the parameterization of the reduced-scale simulation model. Varying the dimensionality of the dependent variable would only affect the scaling required to go from a measured value of λ_{RS} to a corresponding value for λ_{FS} . This means that we can use a single reduced-scale simulation model to deduce relations involving dependent variables of many dimensions, adjusting our only scaling strategy.

3.3.8 Empirical Results

To illustrate some of the issues that arise when building scale models in the manner described here, Figure 1 shows the fractional prevalence resulting from a full-scale individual-based model of a vector borne disease, and similar output from a series of successively smaller reduced-scale models constructed in accordance with the scaling relationships described above. The experimental model was constructed in an agent-based fashion AnyLogic 6 (Advanced Educational Version) and is governed by the parameters shown in Table 1. This model includes interacting populations of individually-represented Vectors (Mosquitoes) and Hosts (People). Transitions (e.g. contracting or recovering from illness) and interactions (e.g. Vector contact with a particular host) are Poisson distributed discrete events, according to transition rates given by the governing parameters.

Despite the stochastic nature of the simulation, the trajectory of prevalence shows a high degree of regularity for human population sizes above 1000. Prevalence curves for the full-scale model and reduced-scale models match closely down to and including a factor of 50x reduction in the human population (population 1000). With populations below this point, however, the results increasingly diverge. We believe that these effects result from the smaller sample sizes coupled with the discrete character of the population interactions.

The empirical results shown here demonstrate the potential for application of the scaling procedure to greatly reduce computational burden of a non-trivial individual-based model. The results do highlight the need to approach interpretation of scale model results with care. Confidence in the results of scale models can be enhanced by performing sensitivity using different scaling levels, in a manner similar to that by which System Dynamics modelers use sensitivity analysis using timesteps to build confidence in the reliability of numerical integration results.

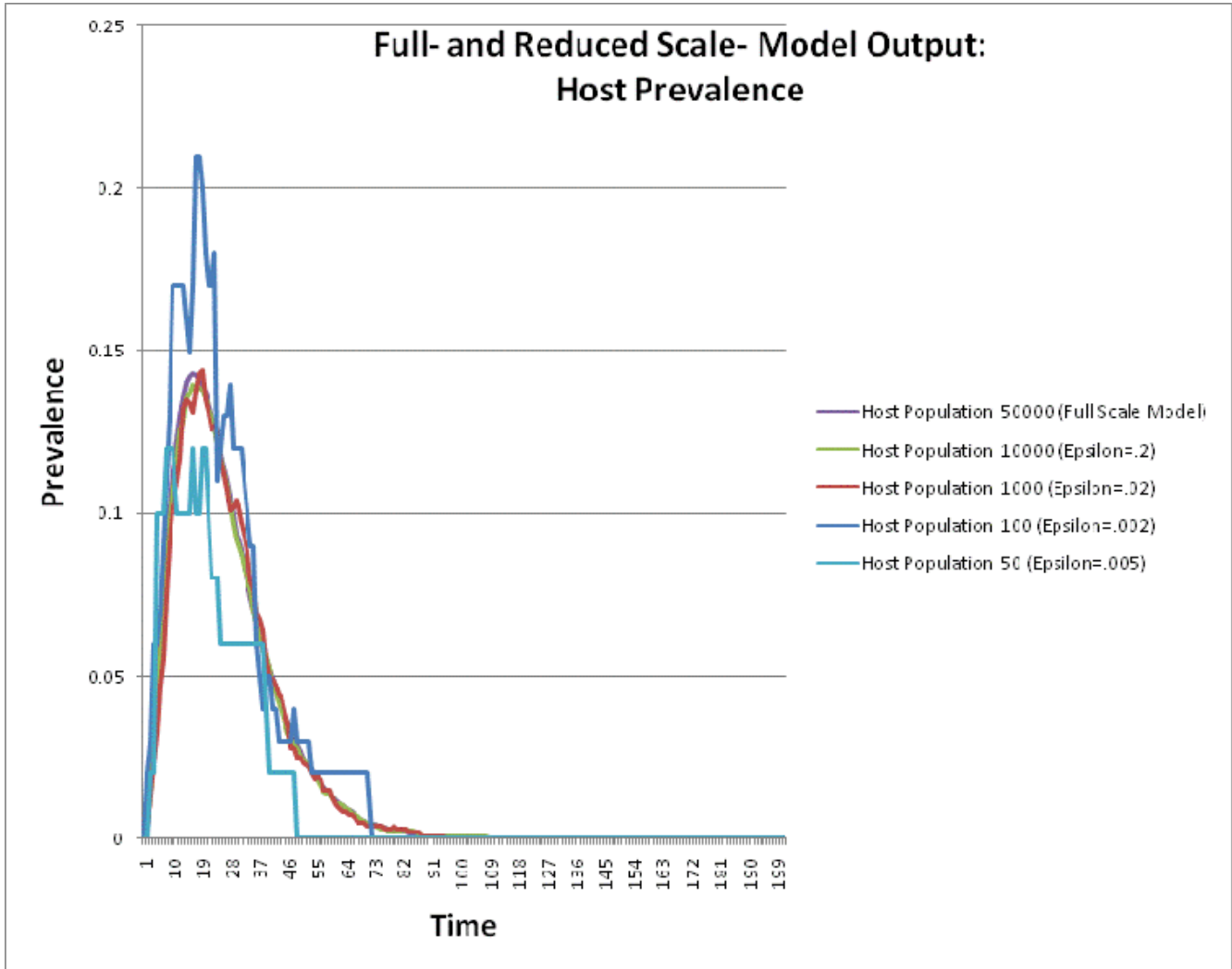


Figure 1: Comparing Results of Full- and Reduced Scale Models. Results show close agreement for Epsilon .02 and above; smaller reduced-scale models exhibit discretization artifacts

3.4 Summary

This section has built on the fact that any dimensionally consistent relations for a dependent variable can be reformulated in a manner that involves only dimensionless parameters, and using a smaller number of parameters are needed than were present in the original system. This reformulated model implicitly defines equivalence classes of *similar* systems such that each dimensionless parameter holds the same value across all members of the equivalence class. We described a (primarily mechanical) process exploits this property of similarity to define reduced-scale individual-based models that yield results that can be precisely scaled up to derive output that would result from a full-scale simulation. This fact is generally used to reason about constructing scale models of systems in the real world, but we have proposed here a novel use of this approach to create reduced-scale models of large-scale individual-based models.

4 A Comment on Heterogeneity

Dimensional analysis has traditionally been applied for continuous physical systems in which a relatively small number of homogeneous parameters (e.g. Young's modulus, density, temperature, etc.) describe the properties of a distributed parameter (e.g. spatially continuous) system. There are compelling reasons for modeling fairly (parameter-wise) homogeneous populations using individual-based models – including the ability to represent non-memory-less processes, multi-scale phenomena, and detailed percolation across networks. Nonetheless, given the strong benefits individual-based models offer for understanding the behavior of heterogeneous populations [1], it is important to consider how the approach presented here extends to such systems.

It is straightforward to apply the approach above for systems exhibiting limited heterogeneity – for example, for individual-based models in which the governing parameter α differs widely across the population. The absence of complications from heterogeneity reflects the fact that although the governing parameters of the individuals may vary in a heterogeneous system, *the dimensions of the governing parameters of different individuals are identical*. Adding limited heterogeneity to a system therefore does not affect the number of *free* governing parameter (Submatrix A by the conventions introduced in the Appendix). The only practical difference caused by addition of limited heterogeneity is that more dimensionless parameters π_j will generally be created. With the exception of any free governing parameters (whose values are directly chosen), all of the heterogeneous parameters of a particular dimensionality will be adjusted in an identical fashion when creating a reduced-scale model.

Consider a variant of our example from the last Section. While we previously assumed that all individuals in the population share values for recovery time (α), assume now that individuals may be associated with any of k distinct values of α_i , $1 \leq i \leq k$. These values all share identical dimensionality $1/Time$. The dimensional set matrix for the heterogeneous system would remain very similar to Figure 2; we would simply replace the column for α with k columns, one for each α_i . Dimensionless parameters π_j would be created for each such governing parameter α_i . Because the dimensions of each α_i governing parameter are identical to that the dimensions of α , the dimensionless parameter associated with each of the new governing parameters would have precisely the same form as did the dimensionless parameter π_2 associated with α .

The situation is only superficially more complex if we consider heterogeneity in a free governing parameter such as β . In such a case, just one of heterogeneous parameters (say, β_{v_i}) would be a free parameter in Submatrix A; all the others would be placed with the bound parameters in Submatrix B (for example, listed just before time t). In accordance with the approach described above, the value of the free governing parameter $\beta_{v_i,RS}$ in the reduced scale model would be freely chosen by the modeler. All other governing parameters β_{v_i} would be associated with dimensionless parameters.

At an operational level, introducing limited heterogeneity does not in general complicate the creation of scale models. The analysis is simply the same as with aggregate parameters; all that is required is systematic scaling of additional governing parameters to realize the scale model.

Despite the mechanical simplicity of reflecting heterogeneity in the analysis, the discrete nature of individual-based models imposes an important limitation. Specifically, the approach presented here assumes that the cardinality of the reduced-scale population is sufficient to maintain the count of heterogeneous parameter classes that were seen in the original system. (In the notation above, it assumes that the population in the reduced-scale model is sufficiently large to represent all k heterogeneous values.) For example, this approach should work fine if there were 100 (k) different values of α_i in both a full-scale population of 10^6 and in a reduced-scale population of 10^3 . Such straightforward scaling will not be possible if we make use of a reduced-scale model with a population size that is too small to represent the heterogeneity in the full system (for example, a reduced-scale population size of 50 if we need to represent 100 different values of parameters), as it will not be possible to associate an individual with each of the reduced-scale parameters. If we wish to consider multiple dimensions of heterogeneity, the reduced-size model would need to be of sufficient size to represent *combinations* of these values.

5 Limitations

This paper has described a rigorous, systematic and surprisingly general approach for deriving a reduced-scale models whose results can be straightforwardly scaled up to yield results representative of a corresponding large-scale model. These approaches draw on the theory of similitude and dimensional scaling that have been extensively exploited in engineering and the applied sciences.

While we believe that the basics of the described approach are sound, the approach is not without some drawbacks and significant research challenges remain for practical application.

Perhaps the biggest challenge was mentioned in the previous section: The use of dimensional scaling for highly heterogeneous populations. Given the strong motivations for using individual-based methods for such populations, it is very important to work to identify systematic means of representing them in reduced-scale models.

A related issue concerns discretization effects. Both theory and empirical observation by the author suggest that the discrete cardinality of populations poses challenges to achieving full similitude with smaller-scale reduced-size models. In addition to heterogeneity scaling concerns, other discretization artifacts can also become pronounced for smaller models. For example, stochastic departures may reflect the fact that as one lowers the size of the reduced-scale population, discrete probabilistic outcomes for the small counts of individuals in reduced-scale model may differ from those of the full-scale model.

6 Conclusion

The System Dynamics community is increasingly applying individual-based models for insight. Such models offer particular value for investigating the effects of targeted interventions and for studying systems with populations exhibiting high heterogeneity, complex and dynamic network structures. Unfortunately, simulation of such models for large populations is often extremely expensive. While it is desirable to gain insight into the behavior of models using reduced-scale populations, naïve construction of such reduced-size models can yield erroneous conclusions. Within this paper, we have described a rigorous, systematic and general technique for building such models.

While the described technique requires further development to address the full richness of modern modeling practice, we believe that it has considerable potential.

More broadly, we believe that dimensional analysis offers many inviting avenues for future research. Specifically, we believe there are high benefits to be gained by applying dimensional scaling theory to model analysis [6]. We believe these benefits are likely to be particularly substantial for individual-based models which are less tractable to closed-form analysis. We believe that the concepts and associated tools of incomplete similitude and intermediate asymptotics [9, 12] hold particular promise for further simplification of dimensional reasoning for individual-based systems. By building on dimensional approaches directly confronting the issue of multi-scale analysis and approximation, renormalization group theory may also be of great value.

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Appendix 1: Derivation of Dimensional Matrix

Section 3.1 described the Buckingham Π Theorem. This theorem shows that any dimensionally homogeneous relation giving the value of a dependent variable x_j in terms of other model parameters can be reformulated as an equation involving only dimensionless parameters Π_i . This section presents a systematic matrix approach for identifying a complete set of dimensionless variables needed for such a reformulation. Interested readers may wish to refer to the more complete exposition of this approach in [8].

The matrix approach is motivated by the fact that in determining the expressions for a particular variable, we are simply selecting the exponent for each governing parameter x_i in that expression. This exercise amounts to solving a set of simultaneous linear equations specifying constraints on the exponents of each governing parameter x_i . The equations are weighted sums of these exponents, reflecting the fact that multiplying variables sums exponents for each dimension, and that raising a governing parameter to a power multiplies all dimensional exponents for that governing parameter by that power. The constraints enforced by these equations reflect the fact that in order to yield dimensionless products, the sum of the exponents associated with each dimension must total to 0.

Following [8], we define 4 matrices, arranged as follows. The dimensions of each matrices are enclosed in parentheses following the matrix name.

		Governing Parameters (x_i)							
		x_1	x_2	x_3	...	x_{n-D}	x_{n-D+1}	...	x_n
Dimensions	d_1	B Matrix ($D \times (n-D)$)					A Matrix ($D \times D$)		
	d_D								
Dimensionless Variables	π_1	D Matrix (Identity; $(n-D) \times (n-D)$)					C Matrix ($((n-D) \times D)$)		
	...								
	π_{n-D}								

Figure 2: Dimensional Set Matrix Structure

Matrices A and B within Figure 2 are to be specified by the modeler. Each entry (i,j) in these matrices specifies the exponent associated with dimension d_i within the dimension product of powers of x_j . Thus, a given column j of matrices A or B represents the exponents associated with each successive dimensions d_i within the dimension of the corresponding governing parameter x_j . For example, if governing parameter x_i were of dimension $\text{Person}^2/\text{Time} = \text{Person}^2 * \text{Time}^{-1}$, the entry in the Person dimension row for x_i would be 2, while that in the Time dimension row would be -1. The entries for any other rows would be 0.

The A and B matrices can be populated by means of a simple dimensional analysis on each governing parameter x_i in turn – where for each such x_i (row) we simply read off the exponent for each dimension (row). The governing parameters chosen for matrix A must be dimensionally independent (in the sense that no product of powers of these governing parameters can be dimensionless), but may be arranged in any order. These parameters are generally those which the modeler believes will have the greatest influence on the dependent variable and those that we wish to explicitly specify for the reduced-scale model. The other parameters can be determined from them.

Entries for matrices C and D have very different meaning than do the entries in A and B. An entry in matrices C and D specifies the exponent associated with a particular *governing parameter* (that associated with the column) within a particular *dimensionless variable* (that associated with the row). Thus a given row of Matrices C and D

specifies the exponents of each governing parameter within the specific dimensionless variable associated with that row. For example, if $\pi_1 = \frac{x_1^2}{x_3 \sqrt{x_4}}$ then the entry for row 1 of C and D would have a “2” in the first column (corresponding to x_1 , a -1 in the 3rd column (corresponding to x_3) and a -1/2 in the 4th column (corresponding to x_4). Matrix D is of fixed structure (the (n-D)×(n-D) Identity matrix) and thus requires no modeler specification.

Matrices A, B and D are all populated directly by the modeler, using previously-known information. By contrast, matrix C must be calculated in order to determine the definitions of the dimensionless variables Π_i in terms of the x_i . Matrix C is calculated from of Matrices A and B. In what amounts to a solving of the implicit set of simultaneous linear equations governing the exponents of the governing parameters, we determine the contents of C as

$$C = -(A^{-1}B)^T$$

It is notable that the A needs to be invertible – hence the requirement for the dimensional independence of the governing parameters of A.

Once matrix C is determined, the definition of each dimensionless variable as a product of powers of the governing parameters x_i can be read off from rows of C and D.

It bears emphasizing that the dimensionless variables identified through this analysis are specific to both the set of independent governing parameters chosen (those associated with the columns of matrix A) as well as to the dimensionality of the chosen dependent variable. The choice of the dimensionally independent governing parameters will in general have a large impact on the dimensional variables identified. By contrast, choosing dependent variables of differing dimensionality will only affect⁸ the expression for π_1 .

⁸ Recall that the dimension of the dependent variable is only encoded within the leftmost column of submatrix B. Reflection on the linear algebra involved reveals that this column only influences the topmost row of submatrix C (the row that indicates the other independent governing parameters that play a role in π_1). Thus, the expressions for all dimensionless variables other than π_1 would remain the same. This bears emphasizing, as it means that the value of the Ψ expression will remain the same regardless of the dimensionality of the dependent parameter.

Appendix 2: Derivation of Scaling Relationships

This appendix provides a straightforward and methodical means of deriving the scaling relationships between the bound governing parameters of the reduced-scale and full-scale models (such as those manually derived in 3.3.5.2)

Reflecting on the structure of the dimensional matrix (see Appendix 1, and the example in Table 1), we can recognize that each dimensionless constant π_i is defined as the product of a unique (bound) governing parameter (the diagonal entries in Submatrix D) with some product of powers of the r free variables (the columns in Submatrix C; for the example, c , P_h , and P_v).

Given this pattern, that an equation establishing $\pi_{i,RS}=\pi_{i,FS}$ can be transformed directly into an equation giving the scaling coefficient for the (bound) governing parameter of interest in terms of a product of power of the coefficients by which each relevant free parameter was reduced.

All we need to do to arrive at such an equation is to divide both sides of the equation by the product of powers of the free governing parameters for the reduced-scale model, and by the value of the governing parameter of interest in the full-scale model (all of which we assume to be non-zero). The resulting formula specifies the ratio of the (bound) governing parameter in the reduced-scale and full-scale model (the scaling coefficient of that bound parameter) in terms of the product of powers of the ratio of each relevant free governing parameters in the full- and reduced-scale models (the scaling coefficients for the free parameters).

For example, consider $\pi_2 = \frac{M_h t}{P_h}$. Because we know the value of this dimensionless parameter must be the same in the full- and reduced-scale models, we must have

$$\frac{M_{h,RS} t_{RS}}{P_{h,RS}} = \frac{M_{h,FS} t_{FS}}{P_{h,FS}}$$

Dividing both sides by the product of powers of the relevant free governing parameters in the reduced-scale model and by the value of the bound parameter in the full-scale model ($M_{h,FS}$) yields

$$\frac{M_{h,RS}}{M_{h,FS}} = \frac{\left(\frac{t_{FS}}{t_{RS}} \right)}{\left(\frac{P_{h,FS}}{P_{h,RS}} \right)}$$

But each of the ratios above is something familiar. The ratio on the left represents the factor by which the bound parameter M_h is scaled in the full- and reduced-size models. The ratios on the right are exactly the ratio between full- and reduced-scale magnitudes for each of the free governing parameters – the scaling coefficients such as ε we chose in section 3.3.5.1. For the example, we chose

$$P_{h,RS} = \varepsilon P_{h,FS}$$

$$P_{v,RS} = \varepsilon P_{v,FS}$$

$$t_{RS} = t_{FS}$$

And thus the ratios above are as follows:

$$\frac{t_{FS}}{t_{RS}} = 1$$

and

$$\frac{P_{h,FS}}{P_{h,RS}} = \frac{1}{\varepsilon}.$$

As a result, we can see that the scaling coefficient for the bound parameter M_h is

$$\frac{M_{h,RS}}{M_{h,FS}} = \frac{\left(\frac{t_{FS}}{t_{RS}}\right)}{\left(\frac{P_{h,FS}}{P_{h,RS}}\right)} = \frac{(1)}{\left(\frac{1}{\varepsilon}\right)} = \varepsilon.$$

Because of the structure of the dimensional matrix, the process we have used here is general, and is applicable as long as the free and governing parameters are non-zero.

This approach allows us to write down the scaling coefficient for each bound governing parameter by inspection. Specifically, we can immediately derive the formula for the ratio of a reduced-scale bound parameter to the corresponding full-scale bound parameter by starting with the product of powers of free parameters occurring in on the right hand side of a dimensionless variable and *substituting in the reciprocal of the scaling coefficient for each free parameter wherever that free parameter occurs in that expression.*

Consider, for example, the bound governing parameter M_h , associated with dimensionless parameter $\pi_2 = \frac{M_h t}{P_h}$.

By the procedure we have outlined, the ratio of $\frac{M_{h,RS}}{M_{h,FS}}$ will be given by $\frac{1}{\left(\frac{1}{\varepsilon}\right)} = \varepsilon$.

By the same token, consider

$$\pi_{11} = \frac{cP_v t}{P_h}.$$

Using the same approach, we can write down by inspection the value of the ratio $\frac{c_{RS}}{c_{FS}}$:

$$\frac{\left(\frac{1}{\varepsilon}\right)(1)}{\left(\frac{1}{\varepsilon}\right)} = 1.$$