**Proposed Checklists for use as one develops the model and the data analysis**

These are the in-house checklists used for the UW Model Repository at [www.physiome.org](http://www.physiome.org/)

The pages are: 1.Summary 2.Project file, 3. CODE, 4.Verif, 5. Valid, 6. Uncertainty, 7. Publication

The check list is to be used by the author and two reviewers, before approval for website.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|   | STANDARDS.1.SUMMARY: Summary of Expectations | Auth | Check1 | Ch 2 |
| Group 1: Identification and Description | x |  |  |
|   | 1. Model Name and No: short and long descriptions complete |  | xy |  |
|   | 2. Code completed, checked .mod file, Model runs correctly |  |  | xyz |
|   | 3. Diagrams correct  |  |  |  |
|   | 4. Reference to Publication describing the model |  |  |  |
|   | 5. Context and Purpose of model defined |  |  |  |
| Group 2. Project File: Basic Content: FIGURES and NOTES |  |  |  |
|   | 1. The chosen model solutions tell some story |  |  |  |
|   | 2. The story is around data, figures and parameter sets (All matched) |  |  |  |
|   | 3. The figures and their titles fit story |  |  |  |
|   | 4. Every figure has axes labeled with symbol, name and units |  |  |  |
|   | 5. Figures use Very short tab labels fitting the topic. |  |  |  |
|   | 6. Graphs use same colors and line types for same variable in every figure. |  |  |  |
|   | 7. Sensitivity functions. How to plot. Why useful. Notes. Use same colors. |  |  |  |
|   | 8. Ontology consistent in notation of .mod, Figures and Notes and Par sets |  |  |  |
|   | 9. Notation consistent with diagrams in .mod text and on the Website |  |  |  |
|   | 10. Parameters sets: Description and rationale for each explained in Notes |  |  |  |
|   | 11. Loops: Purposes and settings; parameter set, plus explanation in Notes |  |  |  |
|   | 12. Optimization re data or other model: description, par set, Notes |  |  |  |
| Group 3. Verification methods: See STANDARDS-VERIF for detail |  |  |  |
|   | 1. Under Notes: Check off list for the model file verification |  |  |  |
|   | 2. List variables computed in the MML code that are serving as checks |  |  |  |
|   | 3. Commentary on checks or missing checks |  |  |  |
|   | 4. Numerical Methods chosen and why. In notes.  |  |  |  |
|   | 5. Solution times chosen; delta t chosen; comments |  |  |  |
| Group 4. Validation methods: See STANDARDS-VALID for detail |  |  |  |
|   | 1. Justify initial and boundary conditions in accord with physiology |  |  |  |
|   | 2. List Data provided and fitted by model, and sources. |  |  |  |
|   | 3. Show fits of data in Figures, and optimization results |  |  |  |
|   | 4. Notes defining contents of each situation, figure or par set |  |  |  |
|   | 5. Parameters estimated and evaluated against literature or other |  |  |  |
| Group 5. Uncertainty Quantification: See STANDARDS-UQ for detail  |  |  |  |
|   | 1. Parameters and Variables chosen |  |  |  |
|   | 2. Define Measures of uncertainty |  |  |  |
|   | 3. Plots or contour maps of projected results |  |  |  |
| Group 6: Scientific Publication: See STANDARDS-PUB for detail |  |  |  |
|   | 1. Summary of the science |  |  |  |
|   | 2. References to subsequent publications or alternative models |  |  |  |
|   | 3. Website for public dissemination, commentary and responses |  |  |  |

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| --- | --- | --- | --- | --- |
|   | STANDARDS 2: The PROJECT FILE: code, data, etc. | Auth | 2nd | Note |
| Group 1: Identification and Description | x |  |  |
|   | 1. Model Name and No: short and long descriptions complete |  | xy |  |
|   | 2. Code completed, checked .mod file, Model runs correctly |  |  | xyz |
|   | 3. Diagrams correct  |  |  |  |
|   | 4. Reference to Publication describing the model |  |  |  |
|   | 5. Context and Purpose of model defined |  |  |  |
|  | 6. Provenance: Refs to prior works |  |  |  |
| Group 2. Project File: Basic Content FIGURES and NOTES |  |  |  |
|   | 1. The chosen model solutions tell some story |  |  |  |
|   | 2. The story is around data, figures and parameter sets (All matched) |  |  |  |
|   | 3. The figures and their titles fit story |  |  |  |
|   | 4. Every figure has axes labeled with symbol, name and units |  |  |  |
|   | 5. Figures use Very short tab labels fitting the topic. |  |  |  |
|   | 6. Graphs use same colors and line types for same variable in every figure. |  |  |  |
|   | 7. Sensitivity functions. How to plot. Why useful. Notes. Use same colors. |  |  |  |
|   | 8. Ontology consistent in notation of .mod, Figures and Notes and Par sets |  |  |  |
|   | 9. Notation consistent with diagrams in .mod text and on the Website |  |  |  |
|   | 10.Parameters sets: Description and rationale for each |  |  |  |
|   | 11. Loops: purposes and settings; par set  |  |  |  |
|   | 12. Optimization re data or other model: descrip, par set, Notes |  |  |  |
| Group 3. Verification methods: See STANDARDS-VERIF for detail |  |  |  |
|   | 1. Under Notes: Check off list for the model file verification (X re 10in Gp 3) |  |  |  |
|   | 2. List variables computed in the MML code that are serving as checks |  |  |  |
|   | 3. Commentary on checks or missing checks |  |  |  |
|   | 4. Numerical Methods chosen and why. In notes.  |  |  |  |
|   | 5. Solution times chosen; delta t chosen; comments |  |  |  |
| Group 4. Validation methods: See STANDARDS-VALID for detail |  |  |  |
|   | 1. Justify initial and boundary conditions in accord with physiology |  |  |  |
|   | 2. List Data provided and fitted by model, and sources. |  |  |  |
|   | 3. Show fits of data in Figures, and optimization results |  |  |  |
|   | 4. Notes defining contents of each situation, figure or par set |  |  |  |
|   | 5. Parameters estimated and evaluated against literature or other |  |  |  |
|   |   |  |  |  |
| Group 5. Uncertainty Quantification: See STANDARDS-UQ for detail  |  |  |  |
|   | 1. Parameters and Variables chosen |  |  |  |
|   | 2. Define Measures of uncertainty |  |  |  |
|   | 3. Plots or contour maps of projected results |  |  |  |
| Group 6: Scientific Publication: See STANDARDS-PUB for detail |  |  |  |
|   | 1. Summary of the science |  |  |  |
|   | 2. References to subsequent publications or alternative models |  |  |  |
|   | 3. Website for public dissemination, commentary and responses |  |  |  |

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| --- | --- | --- | --- | --- |
|   | STANDARDS 3: The CODE: formatting, annotating | Auth | 2nd | Note |
| Group 1. Basic requirements |  |  |  |
|  | Code clearly written |  |  |  |
|  | ALL terms expressed using standard nomenclature  |  |  |  |
|  | Ontology used, and if so consistent? |  |  |  |
|  | Sections demarcated (Parameters, variables, Cs, BCs, Equations |  |  |  |
|  | Modular arrangements of code |  |  |  |
|  | Comments on every line? |  |  |  |
|  | Comments on every line? |  |  |  |
|  | Algorithms explained and referenced if needed |  |  |  |
|  | Short and long descriptions precise and concise |  |  |  |
|  | References listed |  |  |  |
|  | Authors, revisors, date and sign contributions |  |  |  |
|  | References for all parameter values |  |  |  |
|  | Descriptions and references for subsidiary models |  |  |  |
|  | Models and graphs all run |  |  |  |
| Group 2. Conservation, Balances, that are appropriate to the model |  |  |  |
|  | Unitary Balance: (units on all variables and parameters) |  |  |  |
|  | Mass balance: (list constituents whose conservation is checked) |  |  |  |
|  | Charge balance: (ion currents, membrane potential) |  |  |  |
|  | Osmotic balance: (volume, total activities, fluxes)  |  |  |  |
|  | Thermodynamic Balance (Haldane constraints on reactions, etc) |  |  |  |
| Group 3. Verification: math of model and solution methods are sound |  |  |  |
|  | Verification checklist complete? |  |  |  |
|  | Limitation spelled out? Solvers OK? |  |  |  |
|  | Range of Independence of step size in space or time |  |  |  |
| Group 4: Summary of Validation: model is physiologically realistic |  |  |  |
|  | Data provided, and fitted by model |  |  |  |
|  | Initial and boundary conditions in accord with physiology |  |  |  |
|  | Parameters justified (sources provided) and evaluated |  |  |  |
|  | Model is predictive, shown to fit other data not used as basis |  |  |  |
|  |  |  |  |  |
| Group 5: Provision of Source Code and Forum for critiques |  |  |  |
|  | Website source from which to download model code and data |  |  |  |
|  | Website or email to accept queries |  |  |  |
|  | Website for public commentary and responses |  |  |  |
|  | References to subsequent publications or alternative models |  |  |  |
| Group 6. Provenance: Antecedents, derivations and dependencies |  |  |  |
|  | Peer-reviewed publication (pdf copy) |  |  |  |
|  | Lineage of the model (list of antecedent models) |  |  |  |
|  | List higher level models using of which this is a component |  |  |  |
|  | Shortcomings |  |  |  |
|  | Future Needs |  |  |  |

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| --- | --- | --- | --- | --- |
|   | STANDARDS.4. VERIFICATION: | Auth | 2nd | Note |
| Group 1: Conservation, Balances | x |  |  |
|   | Unitary Balance: (units on all variables and parameters |  | xy |  |
|   | Mass balance: (list constituents whose conservation is checked) |  |  | xyz |
|   | Other balances: Charge, Osmotic, Thermodynamics. |  |  |  |
|   |  |  |  |  |
| Group 2. Verification Steps. Checking Math and Numerics of Model  |  |  |  |
|   | All terms defined |  |  |  |
|   | Numerical Solutions check analytic. Why Methods chosen. In notes. |  |  |  |
|   | Analytic solutions built into code? |  |  |  |
|   | Equation formats in similar styles, aligned for easy checking |  |  |  |
|   | Dependence on time step defined for particular parameter values |  |  |  |
|   | Dependence on space step defined for particular parameter values |  |  |  |
|   | Optimizer and loop parameters provided |  |  |  |
|   | Different solvers give same results for ODEs |  |  |  |
|   | Different solvers give same results for PDEs |  |  |  |
|   | Implicit equations solved by iteration? Calculation done how? |  |  |  |
|   | Commentary on checks or missing checks |  |  |  |
|   | Solution times chosen; delta t chosen; comments |  |  |  |
|  | List variables computed in the MML code that are serving as checks |  |  |  |
| Group 3: Verification in Data analysis |  |  |  |
|   | Data available, described and adequate as test |  |  |  |
|   | Data units matched by model |  |  |  |
|   | Multiple data sets available |  |  |  |
|   | Behavioral analysis: Can cover a wide range of situations? |  |  |  |
|   | Sensitivity analysis defined for conditions that fit data |  |  |  |
| Group 4. Validation methods: See STANDARDS-VALID for detail |  |  |  |
|   | 1. Justify initial and boundary conditions in accord with physiology |  |  |  |
|   | 2. List Data provided and fitted by model, and sources. |  |  |  |
|   | 3. Show fits of data in Figures, and optimization results |  |  |  |
|   | 4. Notes defining contents of each situation, figure or par set |  |  |  |
|   | 5. Parameters estimated and evaluated against literature or other |  |  |  |
|   |   |  |  |  |
| Group 5. Uncertainty Quantification: See STANDARDS-UQ for detail  |  |  |  |
|   | 1. Parameters and Variables chosen |  |  |  |
|   | 2. Define Measures of uncertainty |  |  |  |
|   | 3. Plots or contour maps of projected results |  |  |  |
|   | 4. Methods verified for full range of Monte Carlo ranges used |  |  |  |
| Group 6: Scientific Publication: See STANDARDS-PUB for detail |  |  |  |
|   | 1. Summary of verification tests in publication? |  |  |  |
|   | 2. Any failures in verification |  |  |  |
|   | 3. Website for public dissemination of verification methods or tests |  |  |  |

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|   | STANDARDS.5: VALIDATION TESTING: | Auth | 2nd | Note |
| Group 1: Identification and Description |  |  |  |
|   | Model Name and No: short and long descriptions complete |  |  |  |
|   | Code verified and runs correctly. See STANDARDS.4VERIF |  |  |  |
|   | Diagrams represent the key elements of the system |  |  |  |
|   | Reference to Publication describing the model |  |  |  |
|   | Context and Purpose of model defined |  |  |  |
| Group 2. Data for Validation testing. FIGURES and NOTES describe validation |  |  |  |
|   | Experimental data available, and described. Reproducible? |  |  |  |
|   | The data are defined, figures and parameter sets (All matched) |  |  |  |
|   | Data figures: Titles appropriate |  |  |  |
|   | Data figures: axes labeled with symbol, name and units |  |  |  |
|   | Figures use very short tab labels fitting topic. |  |  |  |
|   | Graphs use same colors and line types for same variable in every figure. |  |  |  |
|   | Ontology consistent in notation of .mod, Figures and Notes and Par sets |  |  |  |
|   | Notation consistent with diagrams, code, Website, publication |  |  |  |
|   | Parameters sets: Description and rationale for each set of data |  |  |  |
|   | Optimization re data or other model: Opt Choice, par set, Notes |  |  |  |
|   | Loops: purposes and settings; par set  |  |  |  |
|   |  |  |  |  |
| Group 3. Validation evaluation: |  |  |  |
|   | Initial and boundary conditions in accord with physiology? |  |  |  |
|   | List Data provided and fitted by model, and sources. |  |  |  |
|   | Balance checks. (Mass, charge, osmotic, energy) |  |  |  |
|   | RMS error and CV for all data sets. Different data sets comparable? |  |  |  |
|   | Show fits of data in Figures, and optimization results |  |  |  |
|   | Notes defining contents of each situation, figure or par set |  |  |  |
|   | Parameters estimated and evaluated against literature or other |  |  |  |
|   | Parameter correlations not near 1 |  |  |  |
|   | Parameters omitted from optimization? |  |  |  |
|   | Sensitivity functions. How to plot. Why useful. Notes. Use same colors. |  |  |  |
|   | Residuals random or systematic? |  |  |  |
|  |  |  |  |  |
| Group 4. Uncertainty Quantification: See STANDARDS-UQ for detail  |  |  |  |
|   | 1. Parameters and Variables chosen re sensitivities to critical parameters |  |  |  |
|   | 2. Define measures of uncertainty for system overall behavior |  |  |  |
|   | 3. Make choices for contour maps and pdfs of projected results |  |  |  |
|   |   |  |  |  |
| Group 5: Scientific Publication: See STANDARDS-PUB for detail |  |  |  |
|   |  Summary of the Validation criteria and success |  |  |  |
|   |  Weaknesses in validation; parameters/model components undefined |  |  |  |
|   |  Define future expts, model revisions, commentary and responses |  |  |  |

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| --- | --- | --- | --- | --- |
|   | STANDARDS.6. UNCERTAINTY QUANTIFICATION: | Auth | 2nd | Note |
| Group 1: Identification of UQ in data, model, computation, parameters |  |  |  |
|   |  Model Name and No:  |  |  |  |
|   |  Code verified, runs correctly. See STANDARDS.4VERIF |  |  |  |
|   |  Diagrams for UQ evaluation? |  |  |  |
|   |  Reference to UQ approaches and methods |  |  |  |
|   |  Methods chosen here |  |  |  |
| Group 2. DATA UNCERTAINTY: UQ dependence on data |  |  |  |
|   | Experimental data reproducible?  |  |  |  |
|   | Correlation structure in data sets |  |  |  |
|   | Description of data, noise, shapes of pdfs |  |  |  |
|   | Critical missing data that would constrain solutions |  |  |  |
|   | Constraints from literature. Relevance (species, age, sex, etc.) |  |  |  |
|  Group 3. INPUT and ENVIRONMENT UNCERTAINTY |  |  |  |
|   | Variability in ICs, Input fns and assumptions about expt. conditions |  |  |  |
|  Group 4. PARAMETER UNCERTAINTY: |  |  |  |
|   | Sensitivity functions. How to plot. Why useful. Notes. Use same colors. |  |  |  |
|   | Joint sensitivities for partially correlated parameters |  |  |  |
|   | Loops: stepped setting to illustrate behavior  |  |  |  |
|   | Optimization re data: Confidence, descrip, Correl in covariance matrix |  |  |  |
|  | Parameters sets: Description and rationale for each param set, Notes |  |  |  |
|   | Parameters chosen for MonteCarlo. Sensitivities, lit data, constraints |  |  |  |
|   | Magnitudes of effects on systems behaviors (function space) |  |  |  |
|   | Ranges and shapes of parameter pdfs to use in MonteCarlo;  |  |  |  |
|   | Ranges and shapes of cross section through output trajectories |  |  |  |
|   | Selection of region of predicted responses to characterize |  |  |  |
| Group 5. MODEL STRUCTURAL UNCERTAINTY: |  |  |  |
|   | Modules most subject to uncertainty |  |  |  |
|   | Modules insensitive for the particular data sets |  |  |  |
|   | Modules most critical to the need to predict a chosen outcome |  |  |  |
|   | Notes defining contents of each situation, figure or par set |  |  |  |
|   | Relation between parameter and model uncertainties |  |  |  |
|   | Alternative models: Testing by module substitution. Randomized? |  |  |  |
| Group 6. Assessing Uncertainty Quantification:  |  |  |  |
|   | Identify major sources of Uncertainty (data, noise, model, params) |  |  |  |
|   | Meaningfulness and implications of uncertainty |  |  |  |
|   | Potential means of Reducing Uncertainty |  |  |  |
|   |   |  |  |  |
| Group 7: Scientific Publication: See STANDARDS.7.PUB for detail |  |  |  |
|   | UQ as a major goal of the scientific evaluation |  |  |  |
|   | Meaning of observed UQs |  |  |  |
|   | Recommendations re data, models, improving prediction |  |  |  |

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| --- | --- | --- | --- | --- |
|   | STANDARDS.7.PUBLICATION | Auth | 2nd | Note |
| Group 1: Identification, Description, and role of MODEL in the field |  |  |  |
|   | Purpose: to present REPRODUCIBLE SCIENCE with this advancement |  |  |  |
|   | What is the special contribution of the model |  |  |  |
|   | Was model used in experiment design? Analysis? Validation? UQ? |  |  |  |
|   | Context for this work in the field. The science advanced. |  |  |  |
|   | Novel or confirmatory? |  |  |  |
|  | Acknowledgments. Authorship criteria. |  |  |  |
| Group 2: Technical aspects of the paper  |  |  |  |
|   | Abstract, Intro, Methods, Results, Discussion, Acknowledgment, Appendices |  |  |  |
|   | Every figure has axes labeled with symbol, name, units. Clean. No clutter |  |  |  |
|   | Graphs use same colors and line types for same variable in every figure. |  |  |  |
|   | Ontology consistent in notation of .mod, Figures, Notes, Par sets, Website |  |  |  |
|   | Equations complete and match notation |  |  |  |
|   | Parameter and Variable notation: symbol, name, units, description |  |  |  |
|   | Tables of all parameters, initial conditions, steady state or equilibrium condn |  |  |  |
|   | Parameter influences: Loops: purposes and settings; par set FIGURES? |  |  |  |
|   | Optimization re data or other model: description, par set, Notes |  |  |  |
|   | Graphs; confidence limits, data symbols consistent |  |  |  |
|   | OPEN SOURCE site identified (DATA, MODEL in Project file) |  |  |  |
|   | Parameter files and notes for each Figure in the paper? Tested by running? |  |  |  |
| Group 3. The Modeling and the analyses |  |  |  |
|   | Model completely defined, with rationale, provenance,  |  |  |  |
|   | Verification methods: See STANDARDS-VERIF for detail |  |  |  |
|   | Validation methods: See STANDARDS-VALID for detail |  |  |  |
|   | Assessment of validation process and adequacy of data and analysis |  |  |  |
|   | Model variants defined, invalidated, or not invalidated (working hypothesis) |  |  |  |
|   | Comparing with past work: the novelty (doubts and confidence level) |  |  |  |
|   | Uncertainty Quantification: See STANDARDS-UQ for detail. |  |  |  |
|   | Were predictions testable? |  |  |  |
|   | Reproducibility of Modeling and Data analysis |  |  |  |
|   | Discussion of contribution to science |  |  |  |
|   | Future needs defined? |  |  |  |
| Group 4. Scientific Publication |  |  |  |
|   | Journal choice, OPEN SOURCE, freely downloadable |  |  |  |
|   | Site for Supplements, data, code, project files, |  |  |  |
|   | The REP, REPRODUCIBLE EXCHANGE PACKAGE, and the storage site |  |  |  |
|   | Website for public dissemination, commentary and responses |  |  |  |
|   |  |  |  |  |
|   |  |  |  |  |
|  NOTE | Checklists to be checked by Author and 2 checkers |  |  |  |

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