

# SOFTWARE FOR OPTIMAL DESIGN IN POPULATION PKPD: A COMPARISON

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# Language, availability, interface, models...

	<b>PFIM</b>	<b>PFIM Int.</b>	<b>PkStaMP</b>	<b>PopDes</b>	<b>PopED</b>	<b>POPT</b>
Authors	Mentré et al (Paris)	Mentré et al (Paris)	Leonov (US)	Ogungbenro (Manchester)	Hooker/Nyberg /Ueckert (Uppsala)	Duffull (Otago, NZ)
Language	<b>R</b>	<b>R</b>	<b>Matlab</b> <b>CR</b>	<b>Matlab</b>	<b>Matlab</b> <b>FreeMat</b>	<b>Matlab</b>
Available on website	<b>Yes</b>	<b>Yes</b>	<b>No</b>	<b>Yes</b>	<b>Yes</b>	<b>Yes</b>
GUI	<b>No</b>	<b>Yes</b>	<b>Yes</b>	<b>Yes</b>	<b>Yes</b>	<b>No</b>
Library of models	<b>Yes</b>	<b>Yes</b>	<b>Yes</b>	<b>Yes</b>	<b>Yes</b>	<b>Yes</b>
User defined models	<b>Yes</b>	<b>Yes</b>	<b>Yes</b>	<b>Yes</b>	<b>Yes</b>	<b>Yes</b>
Multi response models	<b>Yes</b>	<b>Yes</b>	<b>Yes</b>	<b>Yes</b>	<b>Yes</b>	<b>Yes</b>
			F. Mentré et al., POPE11			2

# Evaluation of information matrix

	PFIM	PFIM Int.	PkStaMP	PopDes	PopED	POPT
Analytical $\partial/\partial x$	Yes	Yes	No	No	Yes	No
Automatic $\partial/\partial x$ (AD)	No	No	No	No	Yes	No
ODE Models	Yes	Yes	Yes	Yes	Yes	Yes
Non-Block FIM	Yes	Yes	Yes	Yes	Yes	No
Full cov matrix $\Omega$	No	No	Yes	Yes	Yes	No
Full cov matrix $\Sigma$	No	No	No	Yes	Yes	No
Inter-occ variability	Yes	No	No	Yes	Yes	No
Designs differ across responses	Yes	Yes	Yes	Yes	Yes	Yes
Discrete covariates and power	Yes	No	No	Yes/ No	Yes	Yes/ No

# Optimisation

	PFIM	PFIM Int.	PkStaMP	PopDes	PopED	POPT
Exact Design	Yes	Yes	No	Yes	Yes	Yes
Continuous Design	Yes	Yes	Yes	Yes	No	Yes
Constraints	Yes	Yes	Yes	Yes	Yes	Yes
Design Structure	Yes	Yes	Yes	Yes	Yes	Yes
'Bayesian' design (ED)	No	No	No	No	Yes	Yes
Sampling Windows	No	No	Yes	Yes	Yes	Yes

# Optimisation (ctd)

	<b>PFIM</b>	<b>PFIM Int.</b>	<b>PkStaMP</b>	<b>PopDes</b>	<b>PopED</b>	<b>POPT</b>
Algorithm	Simplex  Fedorov - Wynn	Simplex  Fedorov - Wynn	Fedorov - Wynn	Simpex  Exchange  Simulated annealing  Fedorov - Wynn	Random Search  Stochastic gradient  BFGS	Simulated annealing  Exchange
Parallel Computing	<b>No</b>	<b>No</b>	<b>No</b>	<b>No</b>	<b>OpenMPI/ MPCT</b>	<b>No</b>

# Conclusion of PoDe 2007 Meeting



## 1. Start a distribution list: PopDesign

- organised by S. Duffull
- to register: <http://lists.otago.ac.nz/listinfo/popdesign>
- to send an email: [popdesign@lists.otago.ac.nz](mailto:popdesign@lists.otago.ac.nz)
- any questions/comments on design in NLMEM and software tools
- answers by all members of PoDe

## 2. All software have ongoing developments...

## 3. Start a comparison of results provided by software

- value of MF (simple and complex examples) for given design
- *Optimal designs*

## 4. *Should we do only one software?*