Efficient Derivative code for data assimilation systems provided by automatic differentiation

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FastOpt

- Founded in February 2000 at Hamburg
- By Ralf Giering and Thomas Kaminski
- One more colleague as of July 2003: Michael Voßbeck
- Two kinds of business:
  -> Develop and provide tools for Automatic Differentiation (AD)/ Adjoint coding
  -> Consulting projects with focus on AD, Inverse Modelling, Data Assimilation
- 16 years of experience in Adjoint coding

TAF

- Compiler tool for Fortran 77-95: successor of TAMC
- Tangent linear and adjoint code from code of underlying model
- Generated code well readable
- Hessian code by applying TAF twice

TAF-Advanced

- Generation of flexible storing/reading scheme for required variables triggered by TAF init and store directives
- Generation of simple checkpointing scheme (Griewank 1992) triggered by combination of TAF init and store directives
- Generation of efficient adjoint (Christianson, 1994, 1998) for converging iterations triggered by TAF loop directive
- TAF flow directives for black-box routines, or to include user provided derivative code (exploit self-adjointness, MPI wrappers, etc...)
- Automatic Sparsity Detection
- Can generate adjoint with restart capability after interruptions (divided adjoint)

Difficulties

- Need TAF directives from user for efficient adjoint and Hessian code
  -> storing vs. recomputation
  -> indicate parallel loops
- Need to avoid complex control flows
  -> simple ones o.k.
  -> need to recode some nested GOTO, CYCLE, ENTRY constructs
- Few restrictions on coding standard
  -> operator overloading
- Need to avoid complex sequences of dynamic memory allocation
- TAF analysis handles array as a whole
  -> incomplete array assignments can cause problems
- Support for parallelisation still basic
  -> Handles the main OpenMP directives
  -> Hand coding of MPI-wrappers required

Performance Examples

Model (ADM reference)	Lines	Lang	TLM	ADM	Ckp	HES
MOM3 (Galanti et al. 02)	50'000	F77	Yes	4,6	2 lev	-
MITGCM (Marotzke et al. 99, Heimbach et al. 02)	100'000	F77	1,8	5,5	3 lev	11.0/1
BETHY (Kaminski et al. 03, Scholze 03)	5'400	F90	1,5	3,6	2 lev	12.5/5
Nav.-Stokes-Solver (Hinze and Slawig 03)	450	F77	-	2,0	steady	-
NSC2KE (Giering et al. 05)	2'500	F77	2,4	3,4	steady	9.8/1
HB_AIRFOIL (Thomas et al. 03)	8'000	F90	-	3,0		-
ARPS (Yang et al. 04) in progress	40'000	F90	2	11,0	2 lev	-

- Lines: total number of Fortran lines without comments
- Numbers for TLM and ADM give CPU time for (model + gradient) rel. to model
- HES format: CPU time for Hessian * n vectors rel. t. forw. model/ n
- 2 (3) level checkpointing costs 1 (2) additional model run(s)

TAC++

- Compiler tool for C(++)
- Same approach as TAF, similar performance:

Model	#lines of code	FUNC [s]	TLM / FUNC	ADM/ FUNC
Roeflux (Cusdin and Muelle	140	6,2E-7	3,3	3,9
2streams (Pinty et al.)	56	4,0E-7	2,5	2,7
TAU-ij (Heinrich et al.)	129	3,0E-3	--	2,6
GasNetOpt (Steinbach)	25	2,4E-7	2,5	2,7

- Work in progress; functionality will be extended "model by model"
- More details in Vossbeck et al. (2004)

TLM/ADM of fvGCM

Joint work with R. Todling, R. Errico, R. Gelaro, and N. Winslow (GMAO)
TLM/ADM generation automated one-click procedure (no modifi. of generated code)

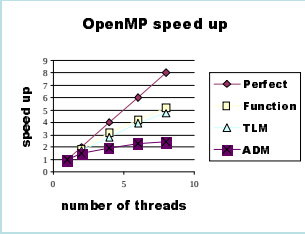
- Storing required variables: 41 TAF init directives and 75 TAF store directives
- 204 TAF flow directives for generation of specific call sequences (e.g. for FFT)
- 11 TAF loop directives to indicate parallel loops
- Complex control flows simplified at two places
- Initialisation split off the main model code
- OpenMP handled by TAF
- ADM MPI wrappers (+2 TLM MPI wrappers) hand-written, interfaces generated by TAF flow directives

More details in Todling et al. (2003) and Giering et al. (2005)

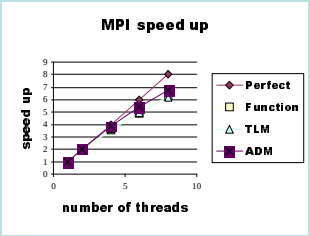
fvGCM Performance

Platform/Setup	TLM	ADM	ADM-noopt
Linux Intel 4	1,5	7.0	-
SGI OpenMP-1 / 8 threads	1,5	10,8	20,6
SGI MPI-1 / 8 processors	1,5	3,9	12,6

- Numbers for TLM and ADM give CPU time for (model + gradient) rel. to model
- Due to bug of SGI-Fortran compiler, flags for full optimisation yields ADM-errors of a few %
- ADM-noopt uses reduced optimisation level for ADM



- Generating code for OpenMP-2 avoid many costly critical sections (verified on Linux; generated code for OpenMP-2 does not run on SGI)



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