Documentation for SimCommand.h and SimCommand.c

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When writing simulation programs, it has proven useful to include a runtime command interpreter in the program so that various commands can be executed at specific times during the simulation. These commands are stored as strings and are passed on to a parser and executer at the proper time. This library contains most of the framework necessary for this interpreter. As a primary use of commands is to output simulation results to text files, the command framework also manages a list of output files.

Header and data structures

The structure cmdstruct, pointed to with cmdptr, contains the information for one command. cmds is a pointer to the superstructure pointer that owns this command. twin is a pointer either from the command template to the command in the queue, or vice versa from the command in the queue to the template. timing is a single character that

represents the command timing rules, of which the options are listed below. on is the time that the command turns on, off is the time that it turns off, dt is the time step between command executions, xt is the time multiplier and is only used if xt > 1. oni, offi, and dti are used instead of on, off, and dt for commands in the integer queue; here, for example, a command is run every dti iterations. invoke depends on whether the command is a template or in a queue; for the template, it is 0 if the command has not been put in a queue and for a command in a queue, it is the number of times that the command has been invoked so far (it equals one during the first command call).

Command execution intervals are never shorter than dt but are sometimes longer than dt because they can only be executed at the times when cmdcheck is called. If $xt \le 1$, the target command times are: on, on+dt, on+2dt, ..., off; if xt > 1, target command times are: on, on+dt, on+xt*dt, on+xt*dt, on+xt*dt, ..., off.

str is the command string. Note that the cmdstruct owns the string, meaning that the string is allocated when a cmdptr is allocated and freed when the cmdptr is freed.

The following elements only apply for commands in a queue and are not used by templates at all. erstr is storage space for an error message that can be passed from the command back to the calling program. There is additional storage space that can be used by the command, although it does not have to be used, which is: i1, i2, i3, f1, f2, and f3; these are all initialized to 0 and keep their values from one command call to the next. Similarly, v1, v2, and v3 are general purpose void* pointers that are initialized to NULL. If memory is allocated for any of these by the command, then the command should also register the address of a function that will free the memory in *freefn. The memory will automatically be freed, using this function, when the command will no longer be executed.

} *cmdssptr;

cmdsuperstruct, which is pointed to by cmdssptr, is a structure that contains lists of runtime commands, the address of a function that is supposed to execute them, and information about the output files and data arrays.

condition is an integer that tells the status of the superstructure. 0 indicates that the data structure is new and/or that it should be fully reinitialized before starting a new simulation. 1 indicates that a simulation is ongoing, but that the time step changed, so all commands in the queue need time updates; also, there may be new commands in the template list that should be added to the queues. 2 indicates that there are new commands in the template list that need to get added to the queues, but that other times don't need updating. 3 indicates that everything is ready to go.

cmdlist is the list of templates for all commands. It has allocated size maxcmdlist and used size ncmdlist. These commands are unsorted and retained even if the simulation is over. These commands are not run from here but are only archived here for copying later into one of the two queues.

cmd is the floating-point (regular) queue of commands, sorted in order of their next exection times. cmdi is the integer queue of commands that are run every iter iterations and for which dt is ignored. In the queues, the object key is the on value of the command and the object item is a pointer to the command structure.

cmdfn is a pointer to the function in the main program that is called to take care of commands (set to docommand for Smoldyn, which is in smolcmd.c). It is sent the argument simvd (void* pointer for the simulation structure), which is unchanged by the routines here, the command, and the command string; see below.

maxfile is the number of allocated file spaces, nfile is the number of output files, root is a root name used before froot, which is another root name and is used for all output files, fname is a list of file names for the various output files, fsuffix is a list of file name suffixes, and fptr is a list of file streams for the output files. Complete file names are a concatenation of root, froot, the file name, and the suffix if there is one. Usually, root is the directory in which the configuration file is located, and froot is a subdirectory for output results. fappend is set to 0 for each file that should be overwritten and 1 for files that should be appended. Output is printed to the file with precision significant figures. outformat can be either 's' or 'c' to indicate space or comma delimited columns.

Data files are similar to file output, but store data within the command superstructure rather than in files and are somewhat simpler. There are ndata arrays stored here, of a total of maxdata that are allocated, each in a list called data and given a name that is stored in dname. These data are only accessible, at present, through the libsmoldyn interface. They are stored as a matrix of doubles, which is appropriate for many data outputs but not ideal for some things, like species numbers and molecule states.

The command superstructure owns all lists and memory pertaining to output files, but cmdfn and simvd are merely pointers that are neither allocated nor freed in this library. flag is simply a number that individual commands can read and/or set, for communication between commands, and is not used in the command handling at all.

Control flow

The function in the main program that takes care of commands is called docommand in Smoldyn. It separates the command string into the first word, which says what the command is, and the rest of the string which contain the parameters for the command, and then it calls the appropriate function to take care of the command. docommand is made available to the SimCommand library by sending its address to scmdssalloc as &docommand during initial structure setup. It is called later on, as needed, by scmdexecute. In this calling, docommand is sent a void* type conversion of sim, which is a structure for the entire simulation parameters and state, a pointer to the command that is to be executed (cmd), and the command string. In this case, the command string is always equal to cmd->str, and so is redundant. However, some commands can invoke other commands directly, in which case they call docommand with a valid string but either the original command or a NULL value for the cmd parameter. This means that all commands need to be able to handle cmd being NULL or the command string in cmd being different from the string in line. For example, the conditional command in Smoldyn called "ifno" first checks the condition and then, if appropriate, it calls docommand with the remainder of the command string.

Command timing

Command timing is encoded in a single character. The list is as follows. The parameters are the values that the user inputs.

code	parameters	execution timing		
?		timing hasn't been set yet		
continuous time queue				
b		runs once, before simulation starts		
а		runs once, after simulation ends		
@	time	runs once, at $\geq time$		
i	on off dt	runs every dt , from $\geq on$ until $\leq off$		
x	on off dt xt	geometric progression		
integer queue				
В		runs once, before simulation starts		
Α		runs once, after simulation ends		
&	i	runs once, at iteration i		
I,j	oni offi dti	runs every dti iteration, from $\geq oni$ to $\leq offi$		
E,e		run every time step		
N,n	n	runs every <i>n</i> time steps		

<u>History</u>

1/10/04 Routines moved to this library from Smoldyn
 1/20/04 Added invoke member to command structure. Also changed declaration of command executing function.

- 1/22/04 Made more changes to the command superstructure, added some functions, and modified others.
- 6/24/04 Changed scmdstr2cmd so that it now allocates the command queue or expands the queue as needed. Also added integer queue stuff to commands and command superstructure and erstr to commands.
- 11/29/06 Added command storage i1, i2, i3, f1, f2, f3, v1, v2, v3, and freefn to command structure.
- 3/12/07 Added xt member to cmdstruct
- 5/25/07 Modified type 'x' command execution
- 11/20/07 Added and implemented enum CMDcode and added scmdcmdtype
- 11/25/07 Replaced all float data types with doubles
- 11/26/07 Added scmdcmdtime
- 4/15/08 Changed scmdexecute with the simut input parameter
- 1/12/09 Added command timing options A, B, &, and I
- 1/14/09 Changed integer queue elements oni, offi, and dti from int to long long int
- 1/19/09 Fixed bugs with long long
- Added dynamic memory allocation to the superstructure for files and rewrote scmdsetfnames, added maxfiles and fappend to superstructure
- 3/27/11 Modified scmdsetfroot
- 4/20/11 Added flag to command superstructure, and functions scmdsetflag and scmdreadflag
- 6/28/11 Added scmdaddcommand
- 4/16/12 Added optional smoldynfuncs.h dependency. This is required for the simLog function. If it isn't present, the library uses printf instead.
 - Edited scmdexecute and scmdoutput to optionally send text to simLog instead of printf.
 - Added type casting to scmdsetfnames for good style and C++ compatibility.
- 7/18/12 Added scmdfprintf function and sigfig element.
- 6/9/15 Added scmdflush.
- 10/6/15 Edited scmdgetfptr to simplify stdout and stderr operation. Fixed some minor bugs in scmdopenfiles, scmdoverwrite, and scmdincfile, all having to do with tests for stdout and stderr.
- 9/10/20 Dilawar had converted scmdfprintf to a C++17 class, but it caused compile errors and didn't add functionality, so I reverted back to the original.
- 12/4/20 Added data element to command structure, rewrote scmdgetfptr, and more updates. These functions now support NULL file pointers (meaning no output).
- 4/13/21 Added cmdlist to the command superstructure and timing to commands. Also added twin and timing to commands and condition to the superstructure. Substantial code overhaul.
- 5/17/21 Renamed cmdfnarg element of cmdsuperstruct to simvd. Also, included it in the SCMDPRINTF macro, so that simulation flags are accounted for during output. Also, exposed scmdalloc and scmdfree to header file.

Utility functions

Internal: void scmdcatfname(cmdssptr cmds,int fid,char *str);

This concatenates all the portions of a file name together, for file number fid, into the string str, which should already be allocated to size STRCHAR. If the total file name is too long, it is truncated at size STRCHAR.

Internal: void scmdcopycommand(cmdptr cmdfrom,cmdptr cmdto);

Copies most elements of cmdfrom to cmdto. This does not copy i1, i2, i3, f1, f2, f3, v1, v2, v3 values or freefn, all of which it sets to either 0 or NULL. It sets invoke to 0 and puts an empty string into erstr. This function sets the twin element of cmdto to point to cmdfrom but it does not change the twin element of cmdfrom. This function is used by scmdupdatecommands for copying commands from their templates to the command queues.

Internal: char *scmdcode2string(enum CMDcode code, char *string);

Converts enumerated command code to a string. string needs to be pre-allocated.

string is returned for easy function nesting.

Memory management

Internal: cmdptr scmdalloc(void);

scmdalloc allocates a command structure, including the string and the error string. The strings are allocated to the fixed size STRCHAR, which is defined in the file string2.h to be 256.

Internal: void scmdfree(cmdptr cmd);
 scmdfree frees a command structure.

cmdssptr scmdssalloc(int (*cmdfn)(void*,cmdptr,char*),void *simvd,char *root); scmdssalloc allocates a minimal command superstructure. cmdfn should be sent in pointing to a function that can execute the commands and simvd is the first argument of that function. For example, in the Smoldyn program, the cmdfn is sent in as &docommand and simvd is sent in as (void*)sim, because sim is a structure that contains all information about the current state of the simulation and is required for most commands. root is the file directory root. The only memory that is allocated is for the superstructure itself. In particular, the command queues are not allocated.

void scmdssfree(cmdssptr cmds);

scmdfree frees a command superstructure and all internal elements except for cmdfn and simvd.

Internal: int scmdcmdlistalloc(cmdssptr cmds,int newspaces);

Expands the cmdlist element of the command superstructure, where the expansion amount is newspaces (which needs to be >0). This creates the initial list if needed. Returns 0 for success or 1 for out of memory.

Internal: int scmdqalloc(cmdssptr cmds,int n);

scmdqalloc allocates the command queue to size n and sets up the queue indexing parameters. It returns 0 for no error, 1 for insufficient memory, 2 for no cmds, or 3 if a queue was already allocated (and thus should not be written over). This function is called by scmdupdatecomamnds.

Internal: int scmdqalloci(cmdssptr cmds,int n);

scmdqalloci allocates the command queue cmdi to size n and sets up the queue indexing parameters. It returns 0 for no error, 1 for insufficient memory, 2 for no cmds, or 3 if a queue was already allocated. This function is called by scmdupdatecommands.

void scmdsetcondition(cmdssptr cmds,int cond,int upgrade);

Sets the command superstructure condition parameter, based on cond and upgrade. If upgrade is 0, then this makes the condition no greater than cond, downgrading it if needed but not upgrading it. If upgrade is 1, this makes the condition no less than cond, upgrading it if needed but not downgrading it. If upgrade is 2, then this simply sets the condition to cond.

int scmdaddcommand(cmdssptr cmds,char timing,double on,double off,double
 step,double multiplier,const char *commandstring);

This adds a command into the cmdlist element (for templates) of the command superstructure with minimal error checking. cmds is the command superstructure and timing is the command code character (see scmdstr2cmd description). on, off, step, and multiplier are the command timing parameters, for when the command should turn on, when it should turn off, its linear timestep, and its exponential multiplier. Finally, commandstring is the actual string of the command. Not all parameters are used for all command types. The function returns: 0 for no error, 1 if memory allocation failed, 2 is cmds was set to NULL, 3 if the commandstring is missing, or 6 if the timing type wasn't recognized. This downgrades the superstructure condition to 2 (or leaves it lower) to indicate that this command needs to be added to a queue.

This takes in a string in line2, parses it for a command type, timing, and command string, and then sends those parameters off to scmdaddcommand to actually add the command. The format of line2 needs to have one of the following forms:

<u>code</u>	parameters	execution timing		
continuous time queue				
b		runs once, before simulation starts		
а		runs once, after simulation ends		
@	time	runs once, at $\geq time$		
i	on off dt	runs every dt , from $\geq on$ until $\leq off$		
Χ	on off dt xt	geometric progression		

integer queue

В		runs once, before simulation starts
Α		runs once, after simulation ends
&	i	runs once, at iteration i
I,j	oni offi dti	runs every dti iteration, from $\geq oni$ to $\leq offi$
E,e		run every time step
N.n	n	runs every <i>n</i> time steps

Returns 0 for success, 1 for failed memory allocation, 2 is cmds was set to NULL, 3 is line2 missing or error in line2 format or command string is missing from line2, 6 if the command timing type character was not one of those recognized.

Internal: void scmddocommandtiming(cmdptr cmd,double tmin,double tmax,double dt)

This inputs a pointer to single command that is already in a command queue, in cmd, and the simulation timing parameters tmin, tmax, and dt. This either computes or recomputes the command timing parameters. It only works with timing parameters for the relevant queue, leaving the others untouched. It also only modifies the timing parameters that weren't set up by scmdaddcommand.

int scmdupdatecommands(cmdssptr cmds, double tmin, double tmax, double dt); As necessary, this copies commands from the template list to the queues, and updates the command timing information. Run this as often as desired, including right before starting a simulation. Returns 0 for success, 1 for failure to allocate memory, or 6 for unknown timing character (a bug). If tmax < tmin or dt ≤ 0, this doesn't do anything but just returns 0, meaning that it's done all it can with the available information, which is nothing.

void scmdpop(cmdssptr cmds,double t); scmdpop removes all commands from the regular queue that are for time t or before, without executing them. The routine can be used after the simulation to avoid executing simulation time commands after an early exit from the simulation loop. It does not do anything to commands in the integer queue.

enum CMDcode scmdexecute(cmdssptr cmds,double time,double simdt,Q_LONGLONG iter,int donow); scmdexecute removes and executes all commands from the command queues that have times that are less than or equal to time for the floating point queue, or

have times that are less than or equal to time for the floating point queue, or iteration counters less than or equal to iter for the integer queue. Integer queue commands are performed first. If iter is set to -1 or less, an internal iteration counter is used; this internal counter starts at 0 and is set to iter any time iter ≥ 0 . simdt is the simulation time step; it is used so that floating point queue commands are executed no more often than once per simulation time step. Commands that should be repeated in the future are put back in the proper queue with the execution time or iteration updated to the previous requested value plus the command time step and with the invoke member incremented. The return value codes are essentially the same as those that are returned from the command executing function given in cmdfn. It is the largest of the errors that are returned from cmdfn: CMDok, CMDpause, CMDstop, CMDwarn, or CMDabort. If the return value is CMDwarn, an

error message is sent to stderr that says which command failed as well as what the error string contains if it was used. This function sends all commands to the command function listed in cmdfn. donow is a flag that produces normal operation, described above, when it equals 0; when it is 1, all remaining commands in the queue are executed immediately and are not put back in the queue.

enum CMDcode scmdcmdtype(cmdssptr cmds,cmdptr cmd);

Assuming command execution function, as well as the individual command functions, are set up for this purpose, this returns the type of command that cmd is. The calls the command execution function with line equal to the command word followed with the word "cmdtype". Commands are supposed to return the appropriate enumerated type. Possible return codes are CMDnone, CMDcontrol, CMDobserve, and CMDmanipulate.

void scmdoutput(cmdssptr cmds);

scmdoutput displays the output files, data arrays, the queue of commands, and the command timing parameters to stdout.

void writecommands(cmdssptr cmds,FILE *fptr,char *filename);

This prints the contents of the command superstructure and the individual commands to fptr using a format that can be read in by Smoldyn, taking the commands from the command list, not from the queues. Items not written to the file are: the iter counter and the root string in the superstructure, and the invoke and internal data of individual commands. filename is optional; if it is included, the printed line for output_files will not include any file called filename. This way, one can run a saved simulation file without immediately overwriting the new configuration file.

void scmdsetflag(cmdssptr cmds,double flag);
 Sets the command superstructure flag value to flag.

double scmdreadflag(cmdssptr cmds);

Returns the command superstructure flag value.

double scmdsetcondition(cmdsssptr cmds,int condition);

Sets the superstructure condition value to the number given here. The system is that it's 0 if the commands are not in the queues yet, or if the ones in there are out of date (e.g. the time step was changed but commands have not been re-enqueued yet), and 1 if the commands are in the queue and are ready to go.

void scmdsetprecision(cmdssptr cmds,int precision);

Sets the precision. Use a negative number for automatic and a positive number for that precision.

int scmdsetoutputformat(cmdssptr cmds,char *format);

Sets the output format. Reads a string in format, which should be either "ssv" or "csv". In the former case, this sets the outformat element to 's' and in the latter case, sets outformat to 'c'. Returns 0 for success and 1 for unrecognized string.

Data functions

int scmdsetdnames(cmdssptr cmds,char *str);

This inputs a list of data names in str as words separated by spaces and creates a new empty data array for each one. This updates the ndata, maxdata, and data elements of the data structure as needed.

void scmdappenddata(cmdssptr cmds,int dataid,int newrow, int narg, ...); This appends data to the data element that is stored with the command, for observation commands (dataid is the data list number, which comes from scmdgetfptr). Enter newrow as 1 to start a new row in the data table, narg as the number of arguments being entered, and then that many arguments, all of which need to be doubles. This basically just calls ListAppendItemsDDv.

File functions

- int scmdsetfroot(cmdssptr cmds,char *root); scmdsetfroot sets the file root element of the command superstructure to the string that is sent in. The function returns 0 for success or 1 if either cmds or root are NULL.
- int scmdsetfnames(cmdssptr cmds,char *str,int append); scmdsetfnames inputs a list of file names in str as words separated by spaces (if a file name has a space in it, this routine won't recognize the name correctly). Set append to 0 if any existing file contents should be overwritten and to 1 if they should be appended. It counts the number of names in the list, updates the nfile element of the command superstructure, allocates the fname and fptr lists as needed, and copies the names to fname. The files are not opened. The routine returns 0 for success, 1 for inability to allocate memory, 2 for a file name that could not be read, or 4 if cmds is NULL.
- int scmdsetfsuffix(cmdssptr cmds,char *fname,int i); scmdsetfsuffix sets the file suffix number for file name fname to equal the integer given in i. If the file name is not recognized, a 1 is returned to indicate an error; otherwise a 0 is returned. scmdsetfnames has to have been called first.
- int scmdopenfiles(cmdssptr cmds,int overwrite); scmdopenfiles opens any output files that are listed in the nfile and fname elements of the command superstructure. Any files that are open when this function is called are first closed. The complete file name that is opened for each file is the string in the root element of cmds, concatenated with the string in the froot element of cmds, concatenated with the fname string for the file. If the name in fname is "stdout" or "stderr" then the file pointer is set to point to stdout or stderr, respectively. If overwrite is non-zero, any prior file is simply overwritten; otherwise, this routine

looks for existing files and asks the user if any existing files should be overwritten. The function returns 0 for success and 1 for failure, where failure might arise from the user saying that a file should not be overwritten or from the inability to open a file for writing. If a file could not be opened, an error message is displayed to stderr. Upon failure, structures are not freed.

int scmdoverwrite(cmdssptr cmds,char *line2);

scmdoverwrite reads the first word in line2, which is supposed to be a file name, looks for that name in the fname list of file names, closes the file, and reopens it. That way, the file is made empty for overwriting. The function stores the new file pointer in the fptr list of cmds. It returns 0 for success or 1 for file not found, or 2 for failure to open for writing.

int scmdincfile(cmdssptr cmds,char *line2);

scmdincfile reads the first word in line2, which is supposed to be a file name, looks for that name in the fname list of file names, closes the file, increments the file name by one, and opens the new file. The function returns 0 for success, 1 for file not found, and 2 for failure to open new file for writing. The new file pointer is stored in the fptr list of cmds. This is useful for creating file stacks.

This is a utility routine for use by commands that save data to files and/or tabular data tables. It reads the first one or two words from line2 and determines if they are file names or data table names by looking them up in the fname and dname lists in the command superstructure. If they are, then the corresponding file pointer and/or data ID number are returned in fptrptr and dataitptr. Send in outstyle as 1 if only a file name is allowed, 2 if only a data table name is allowed, or 3 if both are allowed; only one word is read from line2 in the former two cases and two words are read from line2 in the latter case. Returns the number of parsed objects, which can be 0, 1, or 2, or returns -1 if the first word is neither a filename nor a data table name.

int scmdfprintf(cmdssptr cmds,FILE *fptr,const char *format,...);
Output commands should use this function for printing output rather than the stdio fprintf function. The reason is that this one edits the format string to reflect the number of significant figures that were requested by the user and that are stored in cmdss->sigfig. This also allows for either comma or space delimiters between entries. If fptr is NULL, then this simply returns without doing anything. Returns the number of characters printed, or a negative value for an error.

void scmdflush(FILE *fptr);
 This simply flushes the file.

Possible improvements

The command string is fixed at 256 characters, which could be too short for some commands. In particular, a reasonable command might be "multicommand" whose

arguments are a list of commands that should be run sequentially. This would allow a block structured command language.

Also, the setflag function could be made a lot more powerful using a broadcast message function.