SimTK 1.5 Workshop Installation and Components

Jack Middleton

September 25, 2008

SimTKcore

- Webpage overview
- Overview of download contents
- Help with installs and compiling examples during break

SimTKcore Webpage

- Documents Link
  - Doxygen docs (also in download)
  - User guides (also in download)
  - Workshop slides
- Wiki : tips, know issues
- Bug tracking, forums
- News : announcements

SimTK - the Simulation Toolkit, part of the Simbios project - Microsoft Internet Explorer

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PROJECT

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Project Administrator

Michael Sherman Contact

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Blanca Pineda Contact

SimTKcore

Overview

The SimTK Core biosimulation toolkit brings together in a robust, convenient, open source form the collection of highly-specialized technologies necessary to building successful physics-based simulations of biological structures. These include: strict adherence to an important set of abstractions and guiding principles, robust, high-performance numerical methods, support for developing and sharing physics-based models, and careful software engineering.

We released SimTK 1.5 in early August and will be hosting a 2-day workshop on it on Sept. 25-26 (see http://simbios.stanford.edu/EventsOfInterest/WorkshopSimTK1.5.htm).

Accessible High Performance Computing

We believe that a primary concern of simulation scientists is performance, that is, speed of computation. We seek to build valid, approximate models using classical physics in order to achieve reasonable run times for our computational studies, so that we can hope to learn something interesting before retirement. In the choice of SimTK technologies, we are focused on achieving the best possible

Project Lead

Jack Middleton Contact

Peter Eastman Contact

Michael Sherman Contact

Internet

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Current SimTK 1.5 Programming APIs
Advanced Programming Guide
Guide to writing your own code to extend SimTK Core
Last Update: Aug 28, 2008
Doxygen Docs, v 1.5
Online SimTK reference manual
Last Update: Aug 08, 2008
Simbody User Guide
Theory and alogrithms used in SimTK multi-body dynamics engine
Last Update: Aug 28, 2008
Simmatrix User's Guide
Introduction to using SimTK's Vector and Matrix classes
Last Update: Aug 28, 2008
SimTK 1.5 Tutorial
Introduction on creating multibody dynamics simulations in SimTK
Last Update: Aug 28, 2008
SimTKlapack Overview
Introduction to using SimTK's LAPACK implementation
Last Update: Aug 28, 2008
SimTKmath User's Guide
User guide for SimTK's numerical methods library
Last Update: Aug 28, 2008
SimTK Molecular Modeling Guide
User guide for SimTK's molecular modeling library: Molmodel
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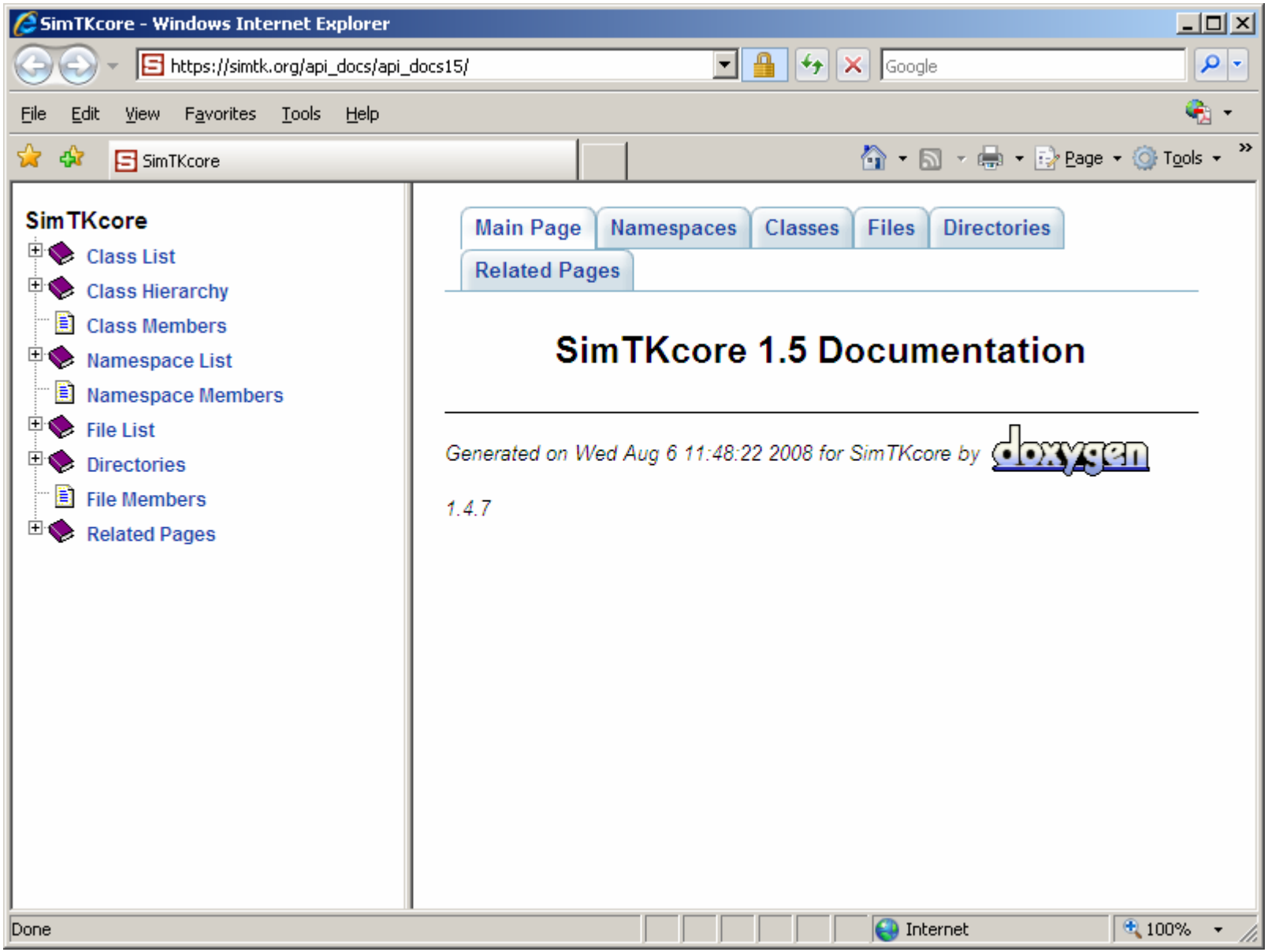
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SimTKcore Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

_DlsMat	
_generic_N_Vector	
_generic_N_Vector_Ops	
_N_VectorContent_Parallel	
_N_VectorContent_Serial	
_SpgmrMemRec	
AbstractValue	*Abstract base class representing an arbitrary val of self-describing type*
AcetylResidue	*Widely used acetyl protein N-terminal end cap*
AdenineBase	
AlcoholOHGroup	***AlcoholOHGroup** is OH group for attachment to aliphatic carbon*
AliphaticCarbon	***AliphaticCarbon** is a tetrahedral sp3 carbon ato for bonding to four other things*
AliphaticHydrogen	***AliphaticHydrogen** is a hydrogen atom for bonding to **AliphaticCarbon** atoms (see below)*
Amber99ForceSubsystem	
AminoAcidResidue	*Amino acid residue building block for protein polypeptide chain molecules*
AminoAcidResidue::Alanine	

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ddress https://simtk.org/api_docs/Simbody/ Go Links

Simbody
Class List
Class Hierarchy
Class Members
Namespace List
Namespace Members
File List
Directories
File Members

Constraint::Ball Class Reference

`#include <Constraint.h>`

List of all members.

Detailed Description

Three constraint equations.

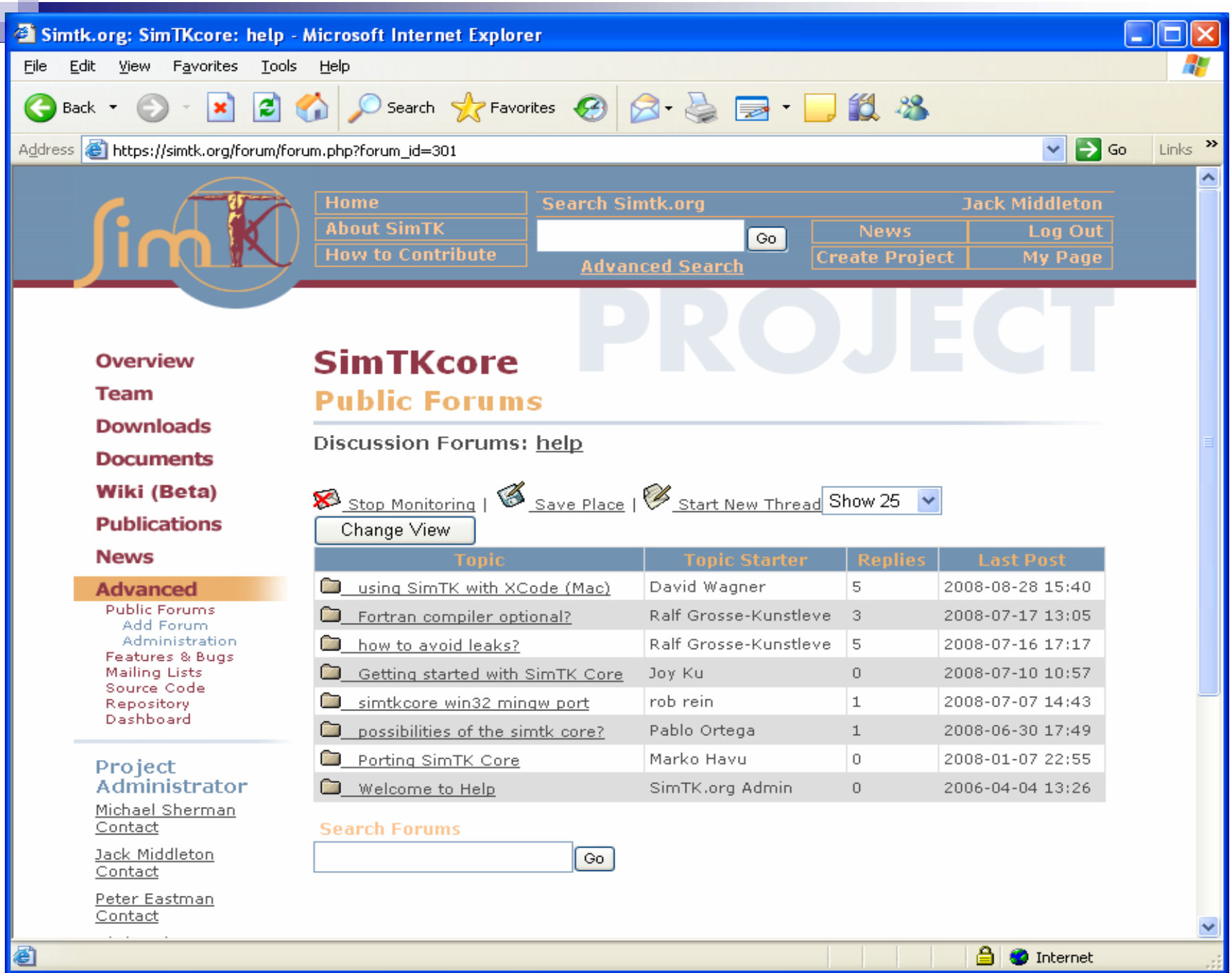
This constraint enforces coincident location between a point on one body and a point on another body.

The constraint is enforced by an internal (non-working) force applied at the spatial location of the point on body 2, on material points of each body that are coincident with that spatial location. Note that this is somewhat asymmetric when the ball is not properly assembled -- it acts as though the contact occurs at the point on body 2, *not* at the point on body 1.

The assembly condition is the same as the runtime constraint -- the two points can be brought together by driving the perr to zero.

Public Member Functions

Ball (MobilizedBody &body1, MobilizedBody &body2)
Ball (MobilizedBody &body1, const Vec3 &defaultPoint1, MobilizedBody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Topic Starter
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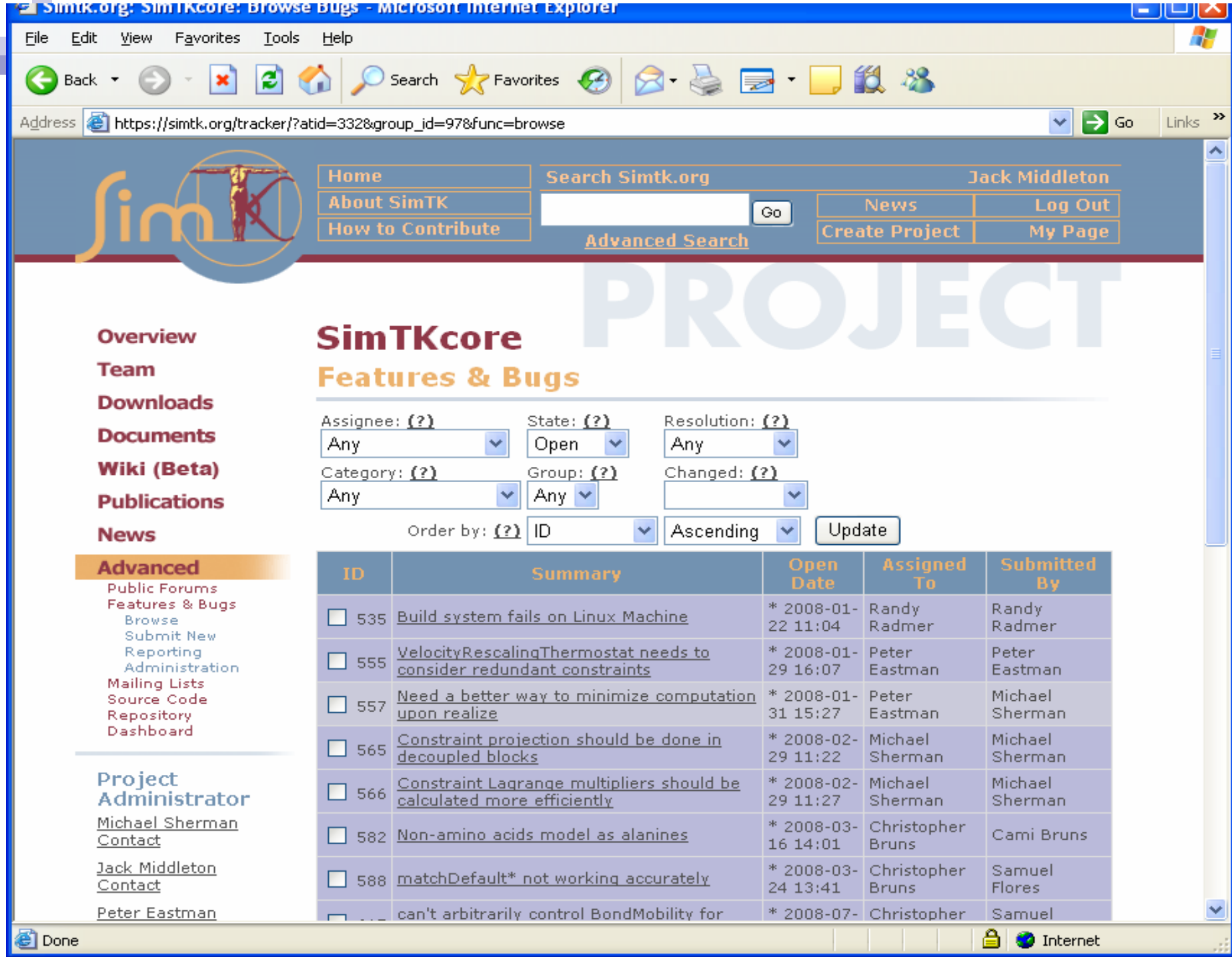
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Dashboard
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Michael Sherman
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Jack Middleton
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State: (?) Open
Resolution: (?) Any
Category: (?) Any
Group: (?) Any
Changed: (?)
Order by: (?) ID
Ascending
Update
ID
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Open Date
Assigned To
Submitted By
535 Build system fails on Linux Machine * 2008-01-22 11:04 Randy Radmer Randy Radmer
555 VelocityRescalingThermostat needs to consider redundant constraints * 2008-01-29 16:07 Peter Eastman Peter Eastman
557 Need a better way to minimize computation upon realize * 2008-01-31 15:27 Peter Eastman Michael Sherman
565 Constraint projection should be done in decoupled blocks * 2008-02-29 11:22 Michael Sherman Michael Sherman
566 Constraint Lagrange multipliers should be calculated more efficiently * 2008-02-29 11:27 Michael Sherman Michael Sherman
582 Non-amino acids model as alanines * 2008-03-16 14:01 Christopher Bruns Cami Bruns
588 matchDefault* not working accurately * 2008-03-24 13:41 Christopher Bruns Samuel Flores
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SimTK core Project Wiki

Tips for SimTK 1.5 Workshop

Cygwin

If you want to run SimTK on cygwin you will need to build your SimTK libraries from so
CMake. Before building SimTK on cygwin you will need to perform the following steps:

1) Install the SimTKlapack libraries for your system from the SimTKlapack project dow

2) Install the SimTKlapack.h from the SimTKlapack project download page and place it
core/include directory. (The SimTKlapack.h in the cpu specific self extracting zip files a

SimTKcore Downloads

- Supported Platforms:
  - Windows XP
  - Mac (Intel)
  - Linux
- Temporarily supported Platforms
  - Mac PPC

Debug vs. Release

Workshop can be done with either

Release is faster

Windows: Release vs. RelWithDebInfo

Linux

Linux

SimTK core software for Linux

1.5.1
August 28, 2008

Patch to SimTK 1.5. Please download and read SimTKcore_README_Linux.pdf for installation instructions.
Release Notes

Download Links

Name	File Type	Platform	Updated
SimTKcore_Debug.sh (99948 kB)	binary	Linux	Aug 28, 2008
Description: Compiled with symbols for debugging.			
SimTKcore_Release.sh (55895 kB)	binary	Linux	Aug 28, 2008
Description: Compiled with full optimization.			

Documentation Links

SimTKcore_README_Linux.pdf (17 kB) Sep 02, 2008
Description: Overview and installation instructions.

Please cite these papers

- Jeanette P. Schmidt, Scott L. Delp, Michael A. Sherman, Charles A. Taylor, Vijay S. Pande, Russ B. Altman, "The Simbios National Center: Systems Biology in Motion," IEEE Transactions on Biomedical Engineering, in press (2008)

- Built on 32bit with gcc 4.1.2

Mac OSX (Intel)

Mac OS X (intel)

SimTK core software for intel based Max OS X. Please see Other Platforms for other MACs/OS.

Download

1.5.1
August 28, 2008

Patch for SimTK 1.5. Please download and read SimTKcore_README_Mac.pdf for installation instructions.
Release Notes

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SimTKcore_Release.dmg (71276 kB)	binary	Mac	Aug 28, 2008
Description: Compiled with full optimization.			

Documentation Links

SimTKcore_README_Mac.pdf (16 kB) Sep 02, 2008
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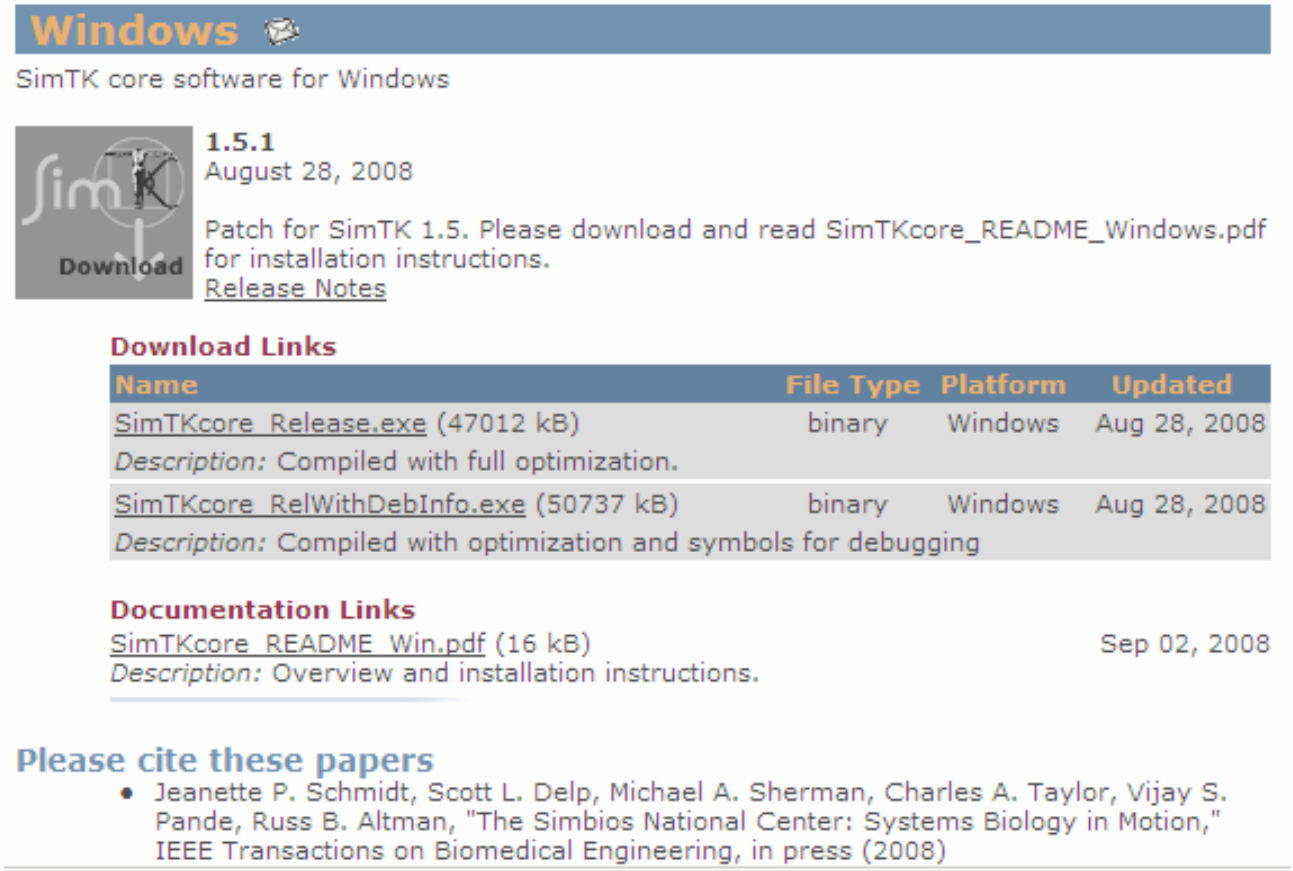
- Xcode 3.0
- Add #include <typeinfo>

Windows XP and Vista



Windows

SimTK core software for Windows

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Release Notes

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SimTKcore_RelWithDebInfo.exe (50737 kB)	binary	Windows	Aug 28, 2008
Description: Compiled with optimization and symbols for debugging			

Documentation Links

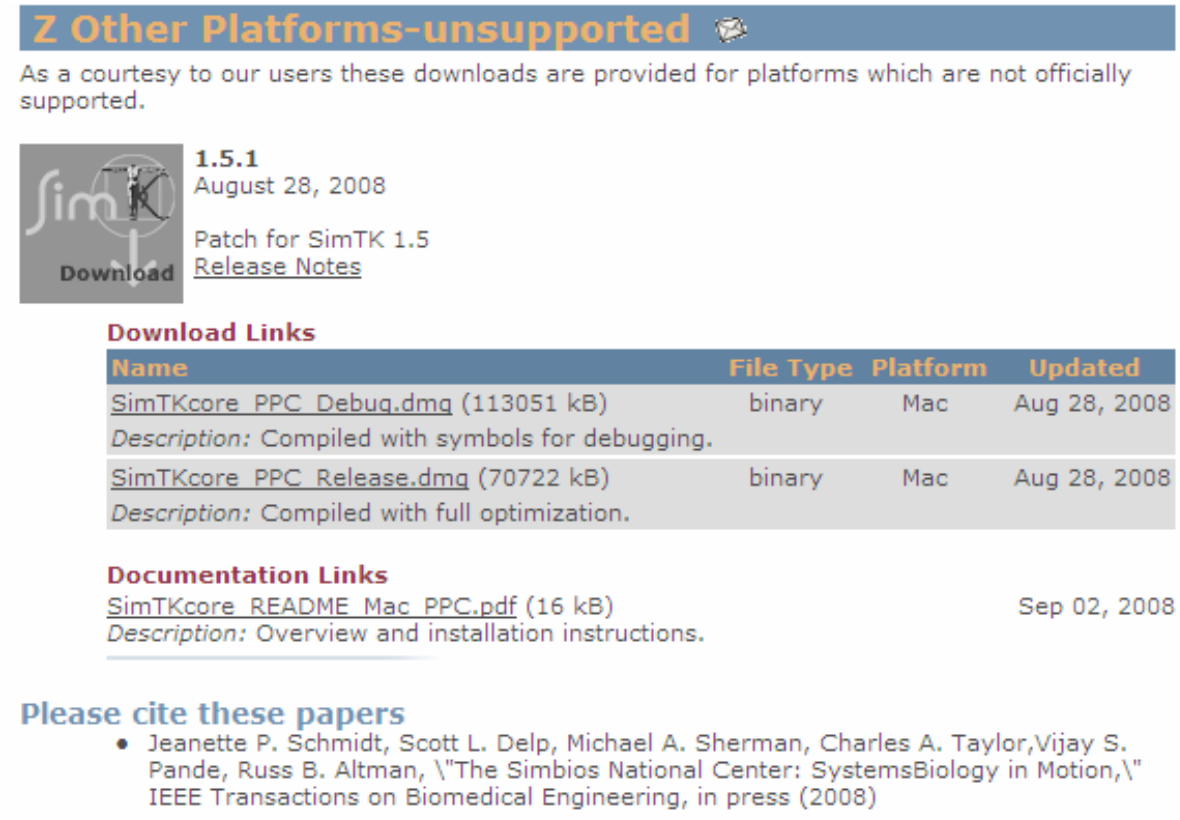
SimTKcore_README_Win.pdf (16 kB) Sep 02, 2008
Description: Overview and installation instructions.

Please cite these papers

- Jeanette P. Schmidt, Scott L. Delp, Michael A. Sherman, Charles A. Taylor, Vijay S. Pande, Russ B. Altman, "The Simbios National Center: Systems Biology in Motion," IEEE Transactions on Biomedical Engineering, in press (2008)

- RelWithDebInfo for debugging

Temporarily Supported Platforms



Z Other Platforms-unsupported

As a courtesy to our users these downloads are provided for platforms which are not officially supported.

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August 28, 2008

Patch for SimTK 1.5
Release Notes

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Description: Compiled with full optimization.			

Documentation Links

SimTKcore_README_Mac_PPC.pdf (16 kB) Sep 02, 2008
Description: Overview and installation instructions.

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- PPC needs libg2c

SimTK and VTK

- Files or directories with “SimTK” in name developed at Stanford (SimTKsimbody.dll)
- Files or directories with “vtk” part of Visualization Tool Kit http://vtk.org (vtkCommon.dll)
- SimTK examples use VTK for graphics but SimTK does not require VTK for simulation

Default Install Locations

Mac: /Developer/SimTK

Windows: C:/Program Files/SimTK

Linux: /usr/local/SimTK

SimTKcore Directory Structure

- SimTK
  - core
    - bin
    - doc
    - examples
    - include
    - lib

Library Naming Conventions

- Debug have “_d” suffix
  - SimTKsimbody_d.dll
- Release and RelWithDebInfo no suffix:
  - SimTKsimbody.dll
- Static linkable libraries have “_static”
  - SimTKsimbody_static_d.lib

SimTK Libraries

- SimTKmolmodel Molecular modeling
- SimTKsimbody_aux VTK interface
- SimTKsimbody Multibody dynamics
- SimTKmath Numerical methods
- SimTKcommon Vector Matrix classes
- SimTKcpodes ODE, DAE solvers
- SimTKlapack Linear Algebra

SimTKlapack

- High speed implementation of LAPACK
  - Threaded for number of cpu's
  - Blocked algorithms for best cache reuse
- Uses ATLAS to generate optimized BLAS
- FORTRAN interface can be called from C/C++.
- #include SimTKlapack.h
- Link to SimTKlapack library

SimTKcpodes

- Multistep, error controlled numerical integrator for multibody dynamics problems
- Advances the ODE, and then performs coordinate projection back to the constraint manifold to exactly solve the DAE
- Joint project between Simbios and LLNL
- Other Integrators available in SimTK (verlet, Runge-Kutta)

SimTKcommon

- System, Subsystem, State
- Vector
- Matrix
- Random (random number generation)
- Rotation, Quaternion
- Event handling
- PolynomialRootFinder

SimTKmath: Nonlinear Optimization

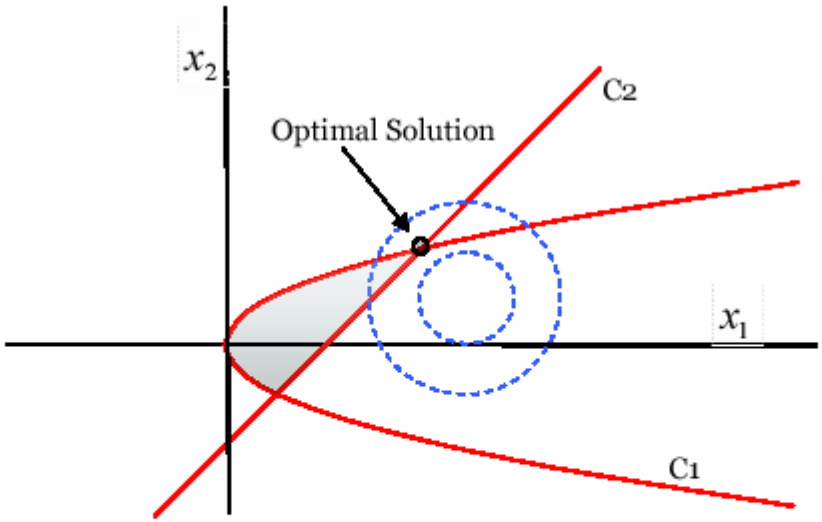

Figure 3: Graph of problem to finding optimal solution to the problem described above. The two constraints are shown in red and the feasible region is show in grey. The contours of the objective function are shown as dashed blue circles.

SimTKmath: Numerical Integration

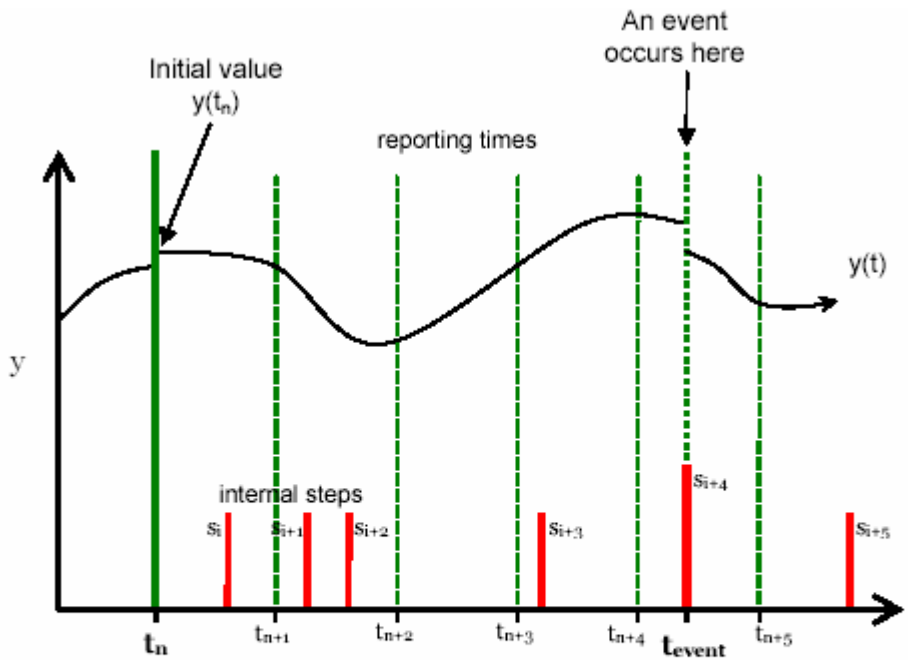

Figure 1: Numerical integration over a continuous segment of a time-stepping trajectory. The continuous region starts at t_n and terminates at t_{event}. Each tall green line represents a return of control to the time stepper: thin dotted ones are caller-requested reporting times; the thick dotted green line is an unrequested return of control just prior to event occurrence and just after event handling.

FactorLU: solve linear systems

$$
\begin{aligned}
x + 2y - z &= 2 \\
4x + 3y + z &= 3 \\
2x + 2y + 3z &= 5
\end{aligned}
$$

$$
\begin{bmatrix} 1 & 2 & -1 \\ 4 & 3 & 1 \\ 2 & 2 & 3 \end{bmatrix}
\begin{bmatrix} x \\ y \\ z \end{bmatrix}
=
\begin{bmatrix} 2 \\ 3 \\ 5 \end{bmatrix}
$$

$$
A \quad x = b
$$

FactorQTZ: Linear Least Squares Solution

- Underdetermined: equations < unknowns

  infinite number of solutions

  find: solution with minimum $|x|_2$

- Over determined: equations > unknowns

  No solution exists

  find: minimum $|Ax - b|_2$

SimTKmath (continued)

Differentiator: Numerical Differentiation

Eigen: Eigen values and Eigen vectors

FactorSVD: Singular value decomposition

SimTKsimbody

- Algorithms and data structures for modeling rigid mulitbody systems in internal coordinates.
- Order(n) algorithm
- Useful for internal coordinate and course grained molecular modeling
- Also for large scale mechanical models like skeletons

SimTKmolmodel

- Molecular modeling layer for Simbody
- Tools for modeling biological macromolecules such as proteins and nucleic acids.
- Dynamics of macromolecules can be simulated using Simbody

Verifying Your Install

- Install checkers in: core/bin
- CoreInstallCheck
  - “Success SimTK has been successfully installed”
- AuxInstallCheck
  - Displays 2 bouncing balls and pendulum

Examples

- Download examples
- Read instructions
- Compile,run

Linux

SimTK core software for Linux

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Tips for Compiling Examples

- Check Wiki
- Windows: release download, MVS configured Release
- Mac: Upgrade Xcode tools
- Linux: gcc 4.1

During Break

- Help with installs
- Help compiling and running examples`