



Multiflash Thermo Package Developments: Support for Multithreaded CAPE-OPEN Clients

Victor Rühle, Francisco Martinez and Richard Szczepanski

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Outline

- Multiflash - introduction
- Motivation for change
- Software development
- Application examples
- Summary

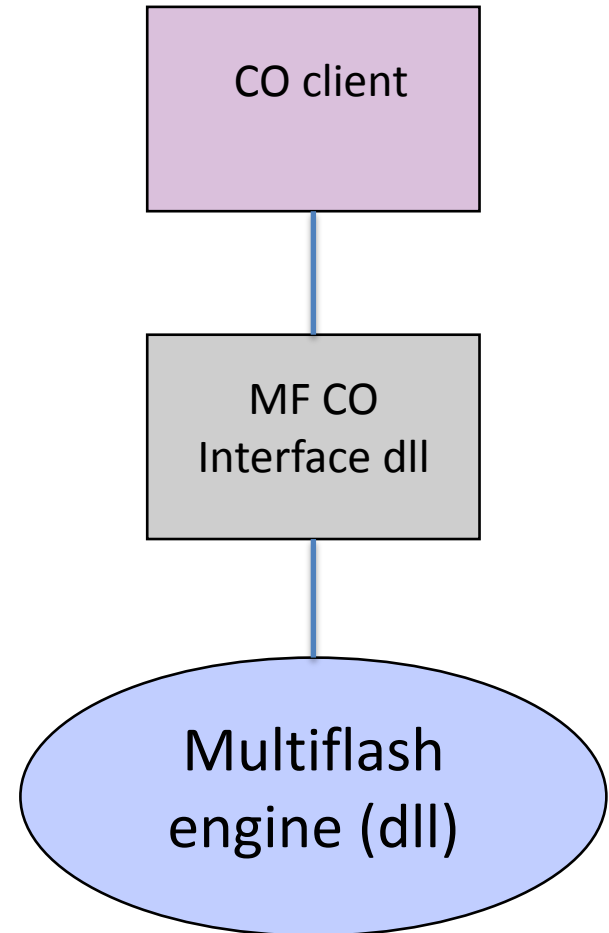


Multiflash: what it does

- Comprehensive PVT and physical properties package
 - Wide range of thermodynamic and transport property models for oil and gas, chemicals, refrigerants etc.
 - Phase equilibria for multiple fluid & solid phases
 - Fluid characterisation based on PVT lab data
- Main applications
 - Production/petroleum engineering
 - Flow assurance engineering
 - Process simulation
 - Equipment/plant design
 - On-line and real time simulation systems and flow-monitoring

Multiflash and CAPE-OPEN

- Supports CO Thermo Spec 1.0 and 1.1
- Includes Property Package Manager and Property Packages with persistence and editing support
- Uses Multiflash GUI to configure PP
- Full multiphase gas/liquids/solids capabilities in the CO 1.1 version
- Supports all (useful):
 - Phases
 - Properties
 - Derivatives
 - Flashes, etc.....





Background

- Multiflash original design 1988/9
 - Total development effort to-date ~ 90 man-years
 - Has proved to be flexible and extensible
 - Mainly Fortran code
- Evolution
 - Fluids
 - Hydrates and pure solids
 - Scales, waxes, asphaltenes
- Current position
 - Widely used in upstream industry with reputation for high quality and excellent support
 - Reliable
 - High performance



Motivation for Change

- Support large simulations
 - Computationally demanding applications, for example
 - Dynamic simulation of pipe networks in OLGA or LedaFlow
 - Large problems – e.g. multiple-refinery optimization in Petro-SIM™, Greater Plutonio life-of-field multi-field network simulation in Maximus™
 - Parametric studies
- Exploit the hardware
 - Multi-processor/multi-core hardware
 - 4, 16, ...128 cores
- Current limitations
 - Static storage
 - limits some applications and leads to large memory requirement
 - Number of components, BIPs and phases
 - Cannot support multiple instances of the calculation routines
 - i.e. is not thread safe
 - Needs locks



Software Development

- Key features
 - Dynamic memory management
 - Thread safe
- Key objectives
 - Compatibility
 - Maintainability
 - Extensibility
 - Reliability
 - Performance

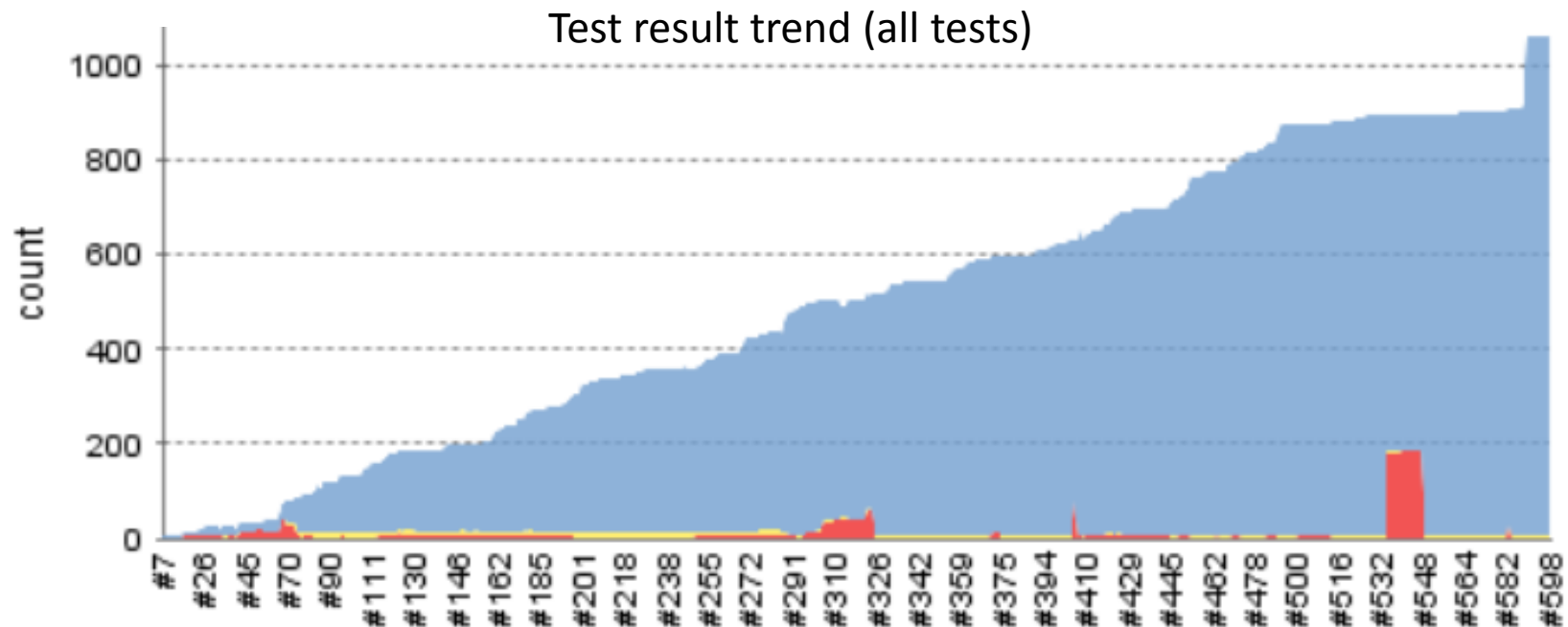


Software Development

- Strategy
 - Redesign using object-oriented approach
 - Decoupled components and code re-use
 - Extensive testing
 - Unit
 - Integration
 - End-to-end
 - Regression
 - Continuous delivery
 - Nightly builds
 - Regular testing in Multiflash GUI
 - Fall-back to MF6 codebase for any features not yet implemented
 - Compatible wrapper interfaces for current API

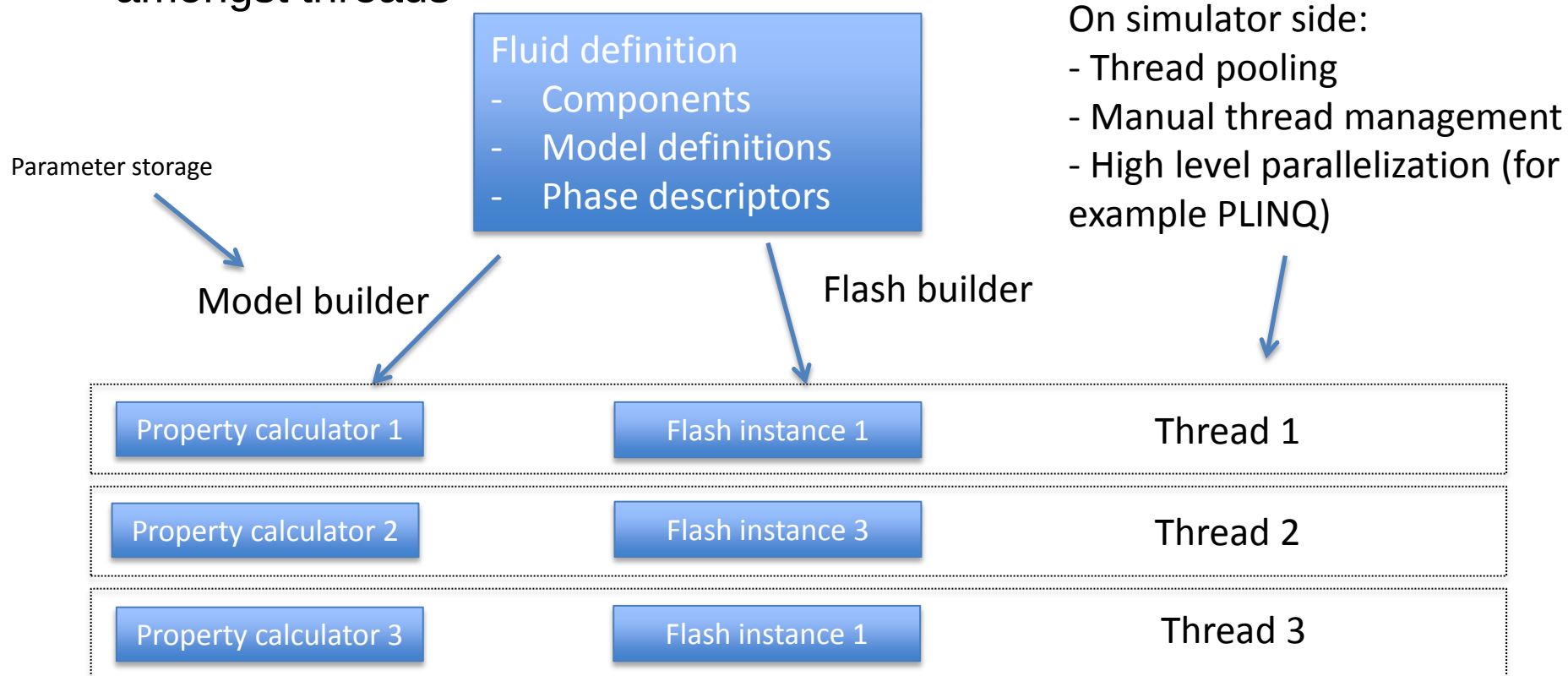
Extensive testing during development

- Testing frameworks
 - Googletest/googlemock
 - python unittest
- Jenkins build server
 - Nightly builds on Windows + Linux



MT concept

- No internal multithreading for flashes
 - Parallelization is responsibility of application, eg. the process simulator
 - Support easy creation of instances which can be distributed amongst threads



Example of API usage (work in progress)

- API must be plain C
 - C++ APIs are compiler dependent (no standard application binary interface)
 - some compatibility within strong limitations
- Simple C api to allow for easy wrapping in higher level languages

Plain C API

```
bool success = mf_flash_create( stream, &flash );
if ( !success ) return false;

success = mf_ptflash_run( flash, 200, 1e6, feed, 1 );
if ( !success ) return false;

int numPhases = mf_flash_get_num_phases( flash );
mf_flash_get_phase( flash, 0, phaseDescriptor,
    phaseType, fraction, composition, ... );

mf_dispose( flash );
```

C# wrapper

```
try {
    var flash = MultiflashWrapper.CreateFlash(stream);

    var result = flash.RunPTFlash(200, 1e6, feed);

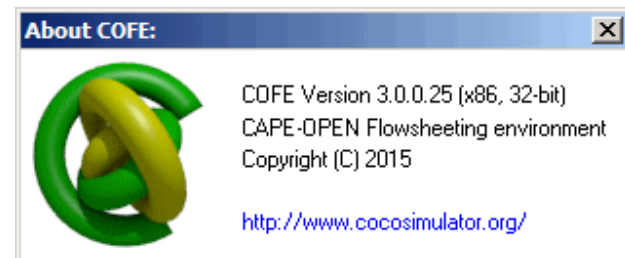
    foreach (var phase in result.Phases) {
        var composition = phase.Composition;
        ...
    }
}
catch (FlashFaileException e) { ... }
```

CAPE-OPEN interface

- Current Multiflash
 - Support for multiple Property Packages (PP) requires locks and unloading/loading of model components
 - Total number of components, models, phases is limited
 - Version 6.0SP1 fixes issue with performance in single threaded mode and crash when running multithreaded
- Multiflash thread safe
 - Removed locks
 - No logical limit on number and size of PPs
 - Not feature-complete so fall-back to MF6
- Comments on the development process
 - Independent testing not straightforward
 - No readily available Material Object code?
 - COFE Version 3.0 used to test the Multiflash PP

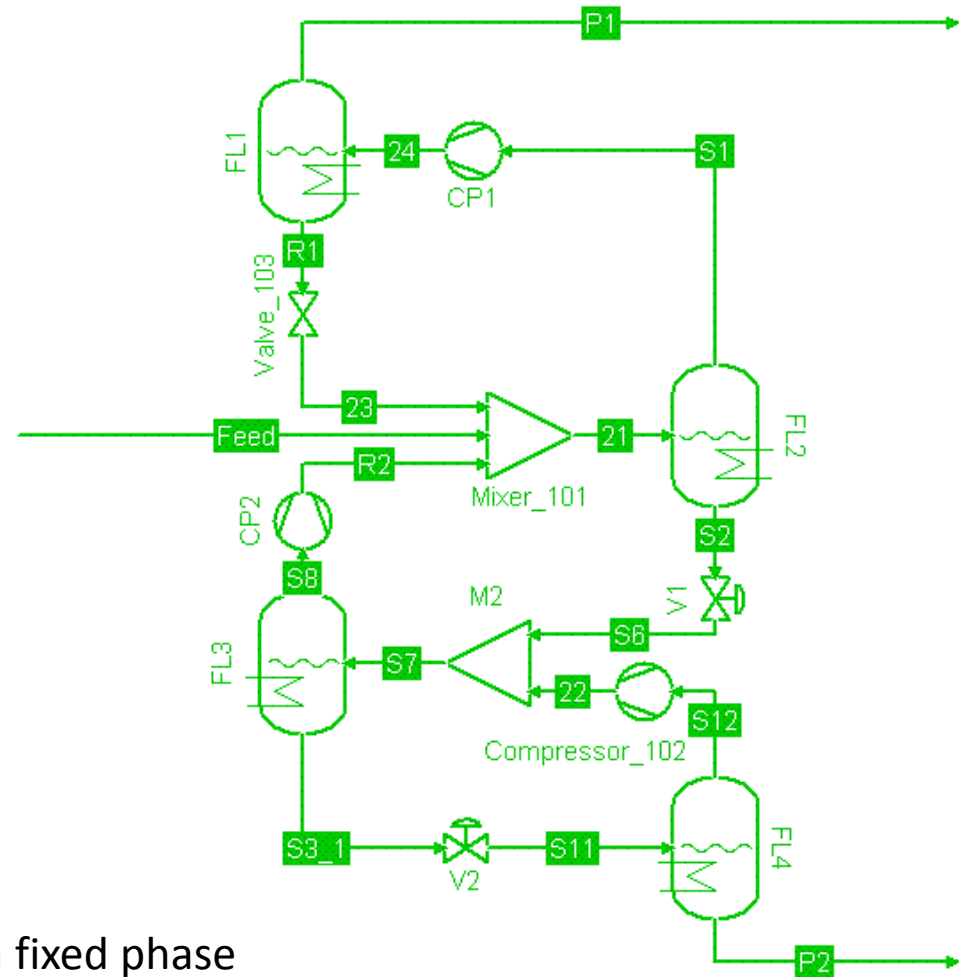
Examples

- Cavett process – COFE
- Refinery light-ends separation with parametric study – COFE
- Flash calculations for complex phase diagram including hydrates and ice
- Timings taken on Core i7-4770 3.4 GHz (4 cores)



Cavett Process - COFE

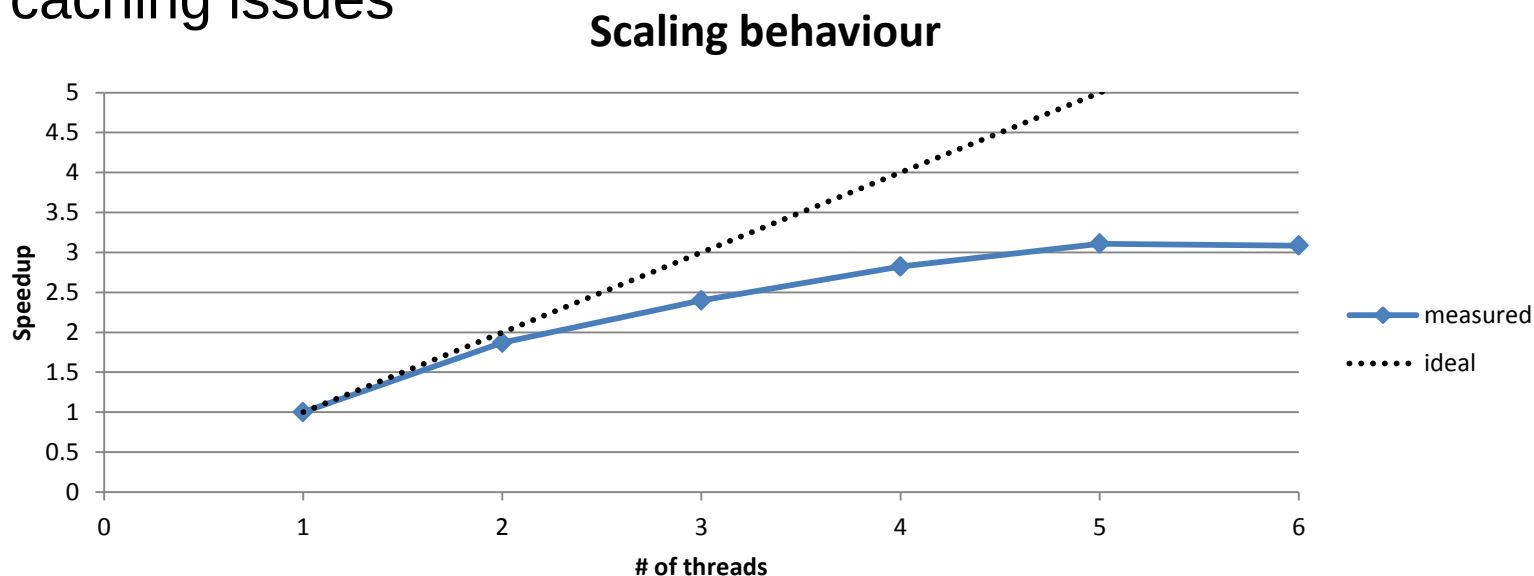
- 16 components
- PR eos
- Phases
 - Vapour
 - Liquid
- Flow sheet solves in ~0.5s, hard to benchmark accurately
- Slight improvement with multiple threads
 - Cost of creating a material objects for each thread?



Bottleneck currently: ~50% time spent in fixed phase fraction flash (bubble point) calculations

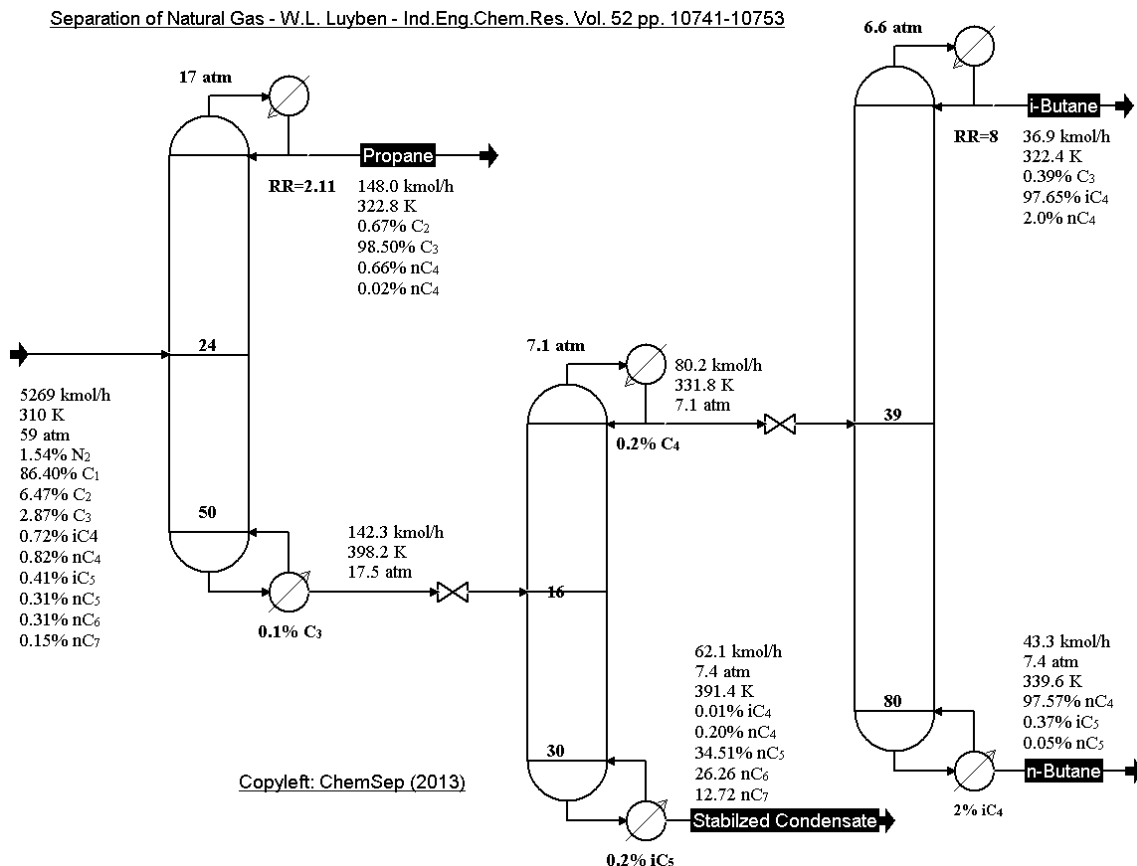
Cavett: Parametric study

- Parametric study
 - T, P in input feed
 - 30x30 points
- Possible reasons for non-ideal scaling
 - GUI updates, competing with other processes, multithreading implementation in COFE, global heap allocator lock, memory caching issues



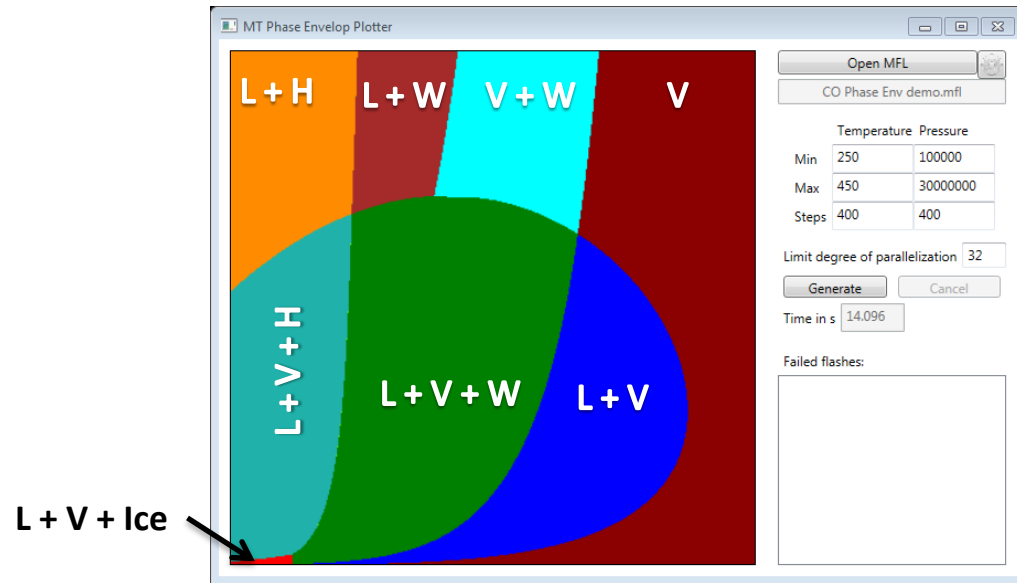
Refinery light-ends separation - COFE

- 10 components
- PR eos
- Phases
 - vapour
 - Liquid
- Solved in ~8s
 - Doesn't seem to be limited by thermo package
- Parametric study speedup 3.8



Phase diagram - Multiflash

- 10 components
- CPA eos
- Phases
 - Vapour
 - HC liquid
 - Water
 - Hydrate II
 - Ice



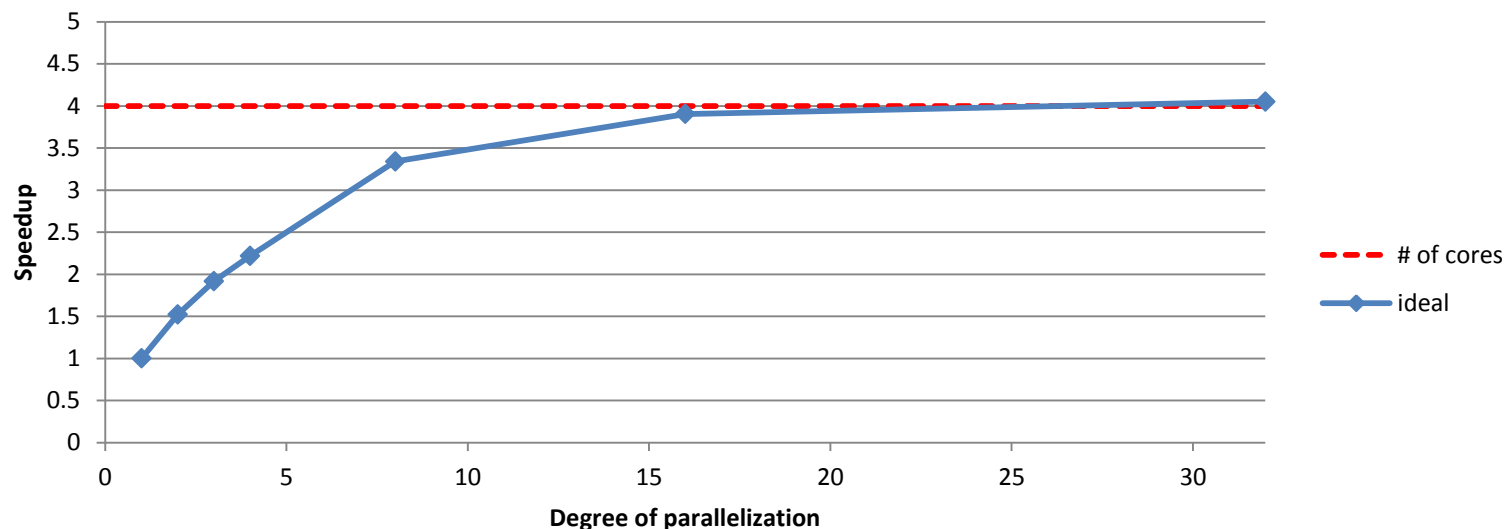
- Trivial to parallelize, high level parallel implementation using .NET PLINQ

```
var slices = from T in temperatures.AsParallel().AsOrdered()
              select singleThreadedSliceCalculationFunc(T);
```

- No manual load balancing or thread/task pooling
- Observed speedup in multithreading up to around 4

Phase envelope multithreading

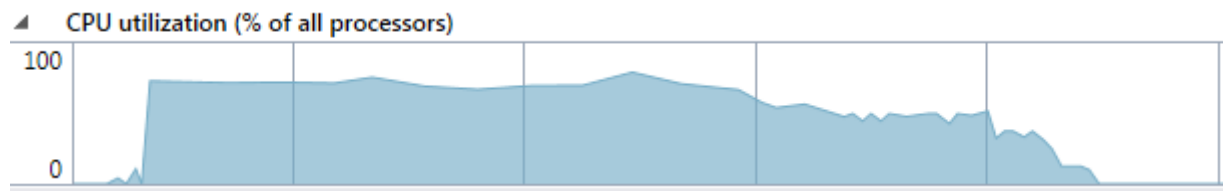
Better speedup with higher level of parallelization than available cores



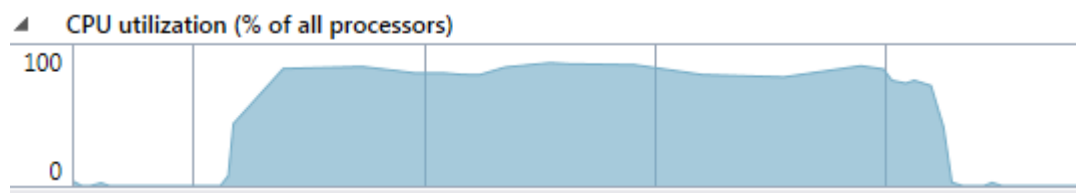
PLINQ degree of
Parallelization (DP)

DP = 8

CPU utilization



DP = 32



Summary

- Multiflash native support for multithreaded applications in 2016
- Improved memory footprint
- Good scaling of CPU performance
 - Performance depends on threading implementation by consumer
- How to test CO interface (automated testing)?
 - .NET code to allow validation of interface and values within standard testing framework (e.g. MSTest, Nunit, xUnit.Net)
- Thanks to Jasper van Baten (amsterCHEM) for help and discussions