

Open Compute Stack (OpenCS)

Overview

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DAE Tools Project,

<http://www.daetools.com/opencs>



What is OpenCS?

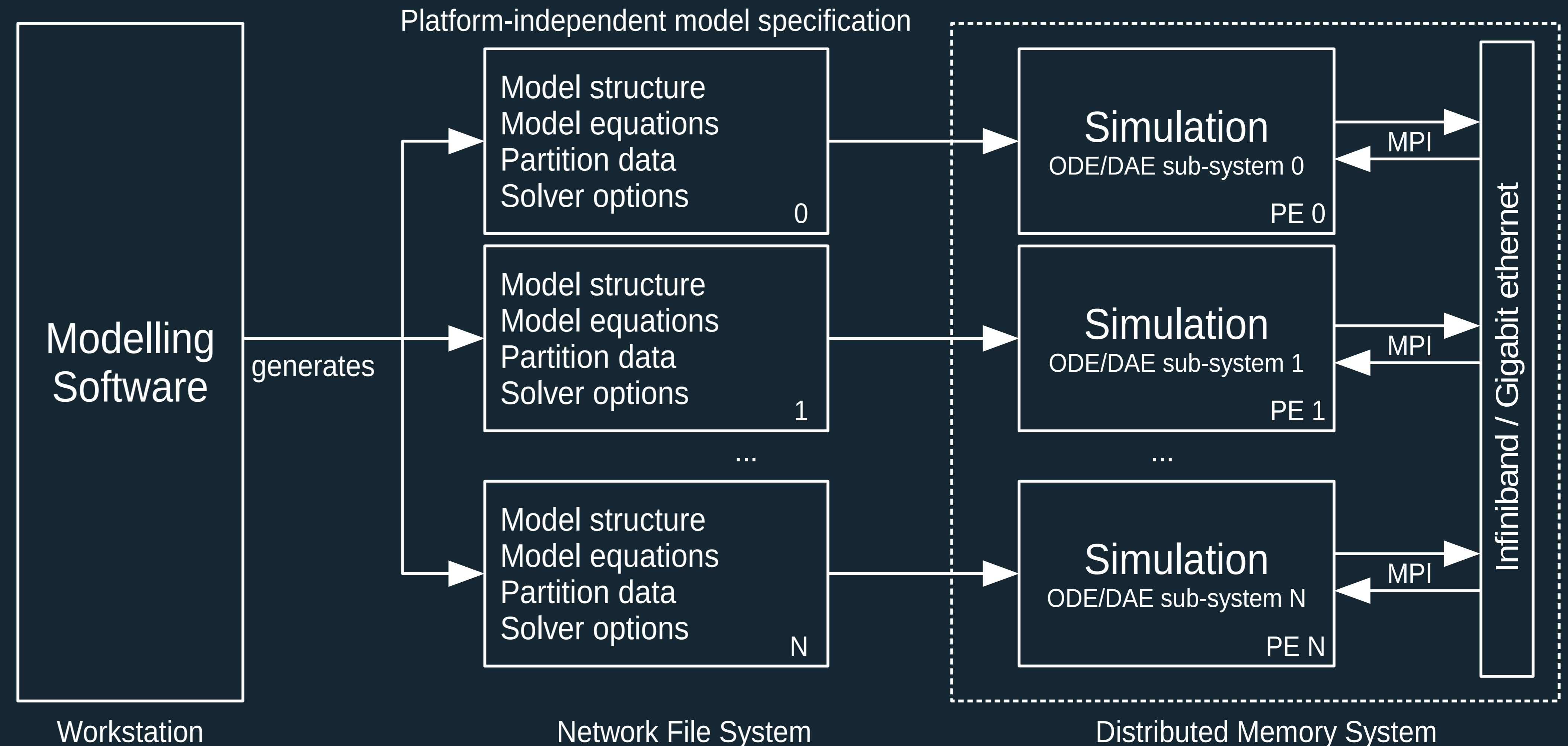
A framework for:

- 1. Equation-based modelling**
(large-scale ODE/DAE systems)
- 2. Parallel evaluation of equations**
- 3. Model exchange**
- 4. Parallel simulation on:**
 - Shared memory systems
 - Distributed memory systems

Multi-domain applications

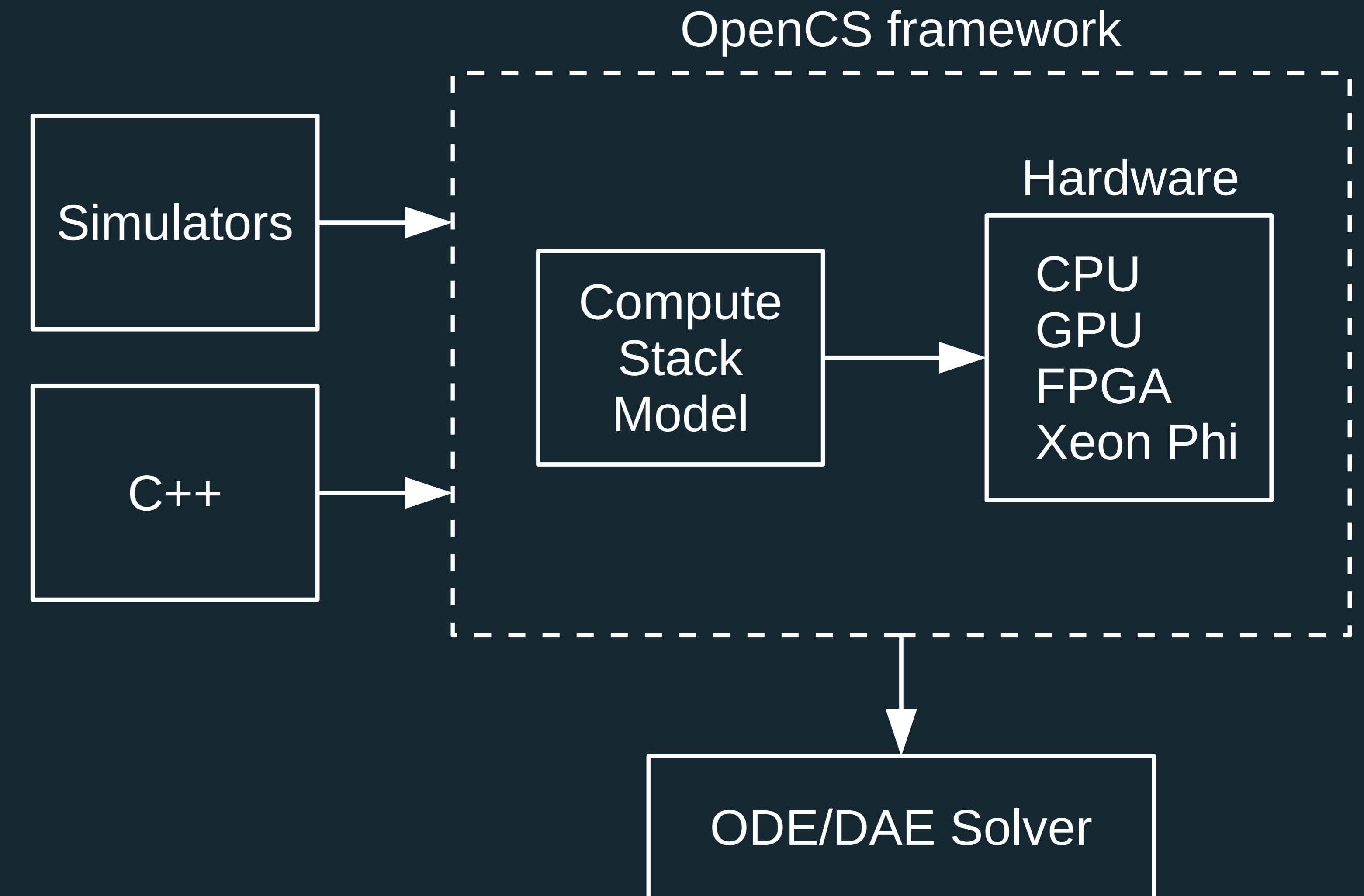
Free/Open source software

Cross-platform



Use case scenarios

1. **Development of large-scale models (C++)**
2. **Parallel evaluation of model equations**
3. **Universal parallel simulations on shared and distributed memory systems**
4. **Model export from simulators for:**
 - Model exchange
 - Benchmark between simulators
 - Benchmark between HPC systems (i.e. hybrid CPU+GPU and CPU+FPGA clusters)



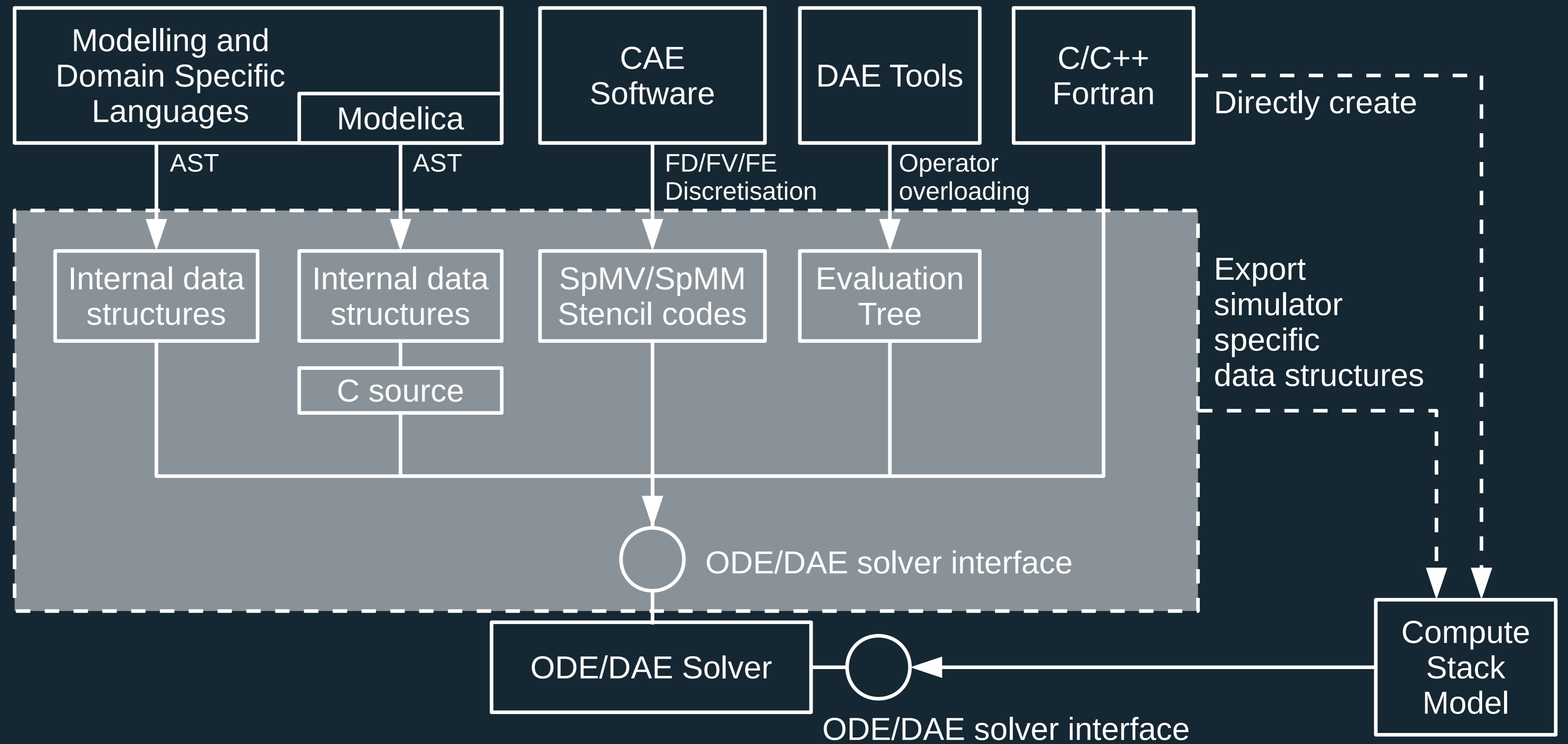
What can be done with OpenCS?

Model specification

- **Direct implementation** in C++
- **Export** from 3rd-party simulators

Model exchange

- **OpenCS models** stored as files in a **platform-independent binary format**
- **The OpenCS API:**
 - Loading the models into a host
 - Interface to ODE/DAE solvers (i.e. evaluation of equations)



What can be done with OpenCS?

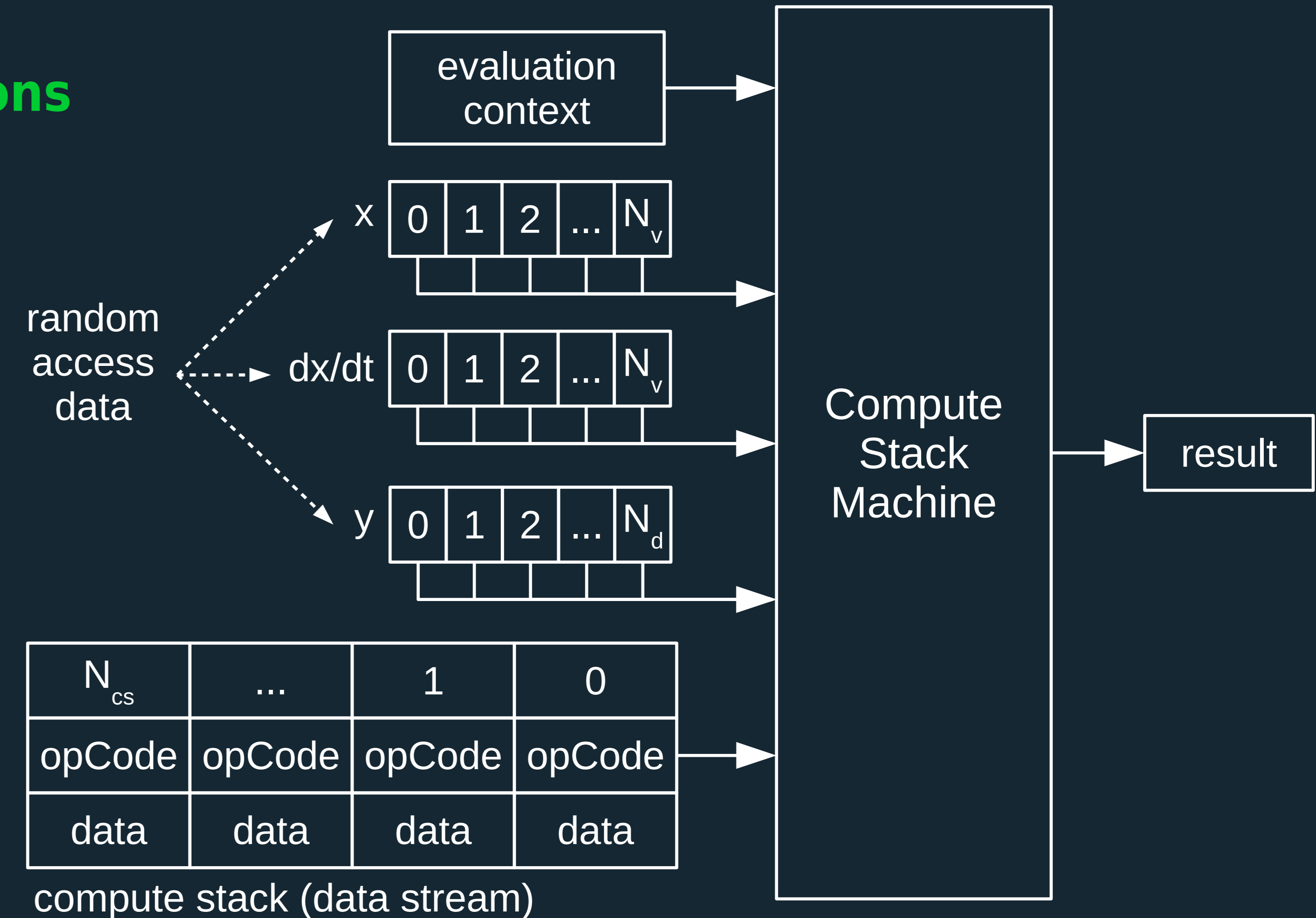
Platform-independent description of model equations

Reverse Polish (postfix) notation (Compute Stack)

Evaluation using a Compute Stack Machine

Advantages:

- Equations as an array of binary data
- Direct evaluation on all computing platforms
- Specialised hardware for evaluation (i.e. FPGA)
- No additional processing nor compilation steps

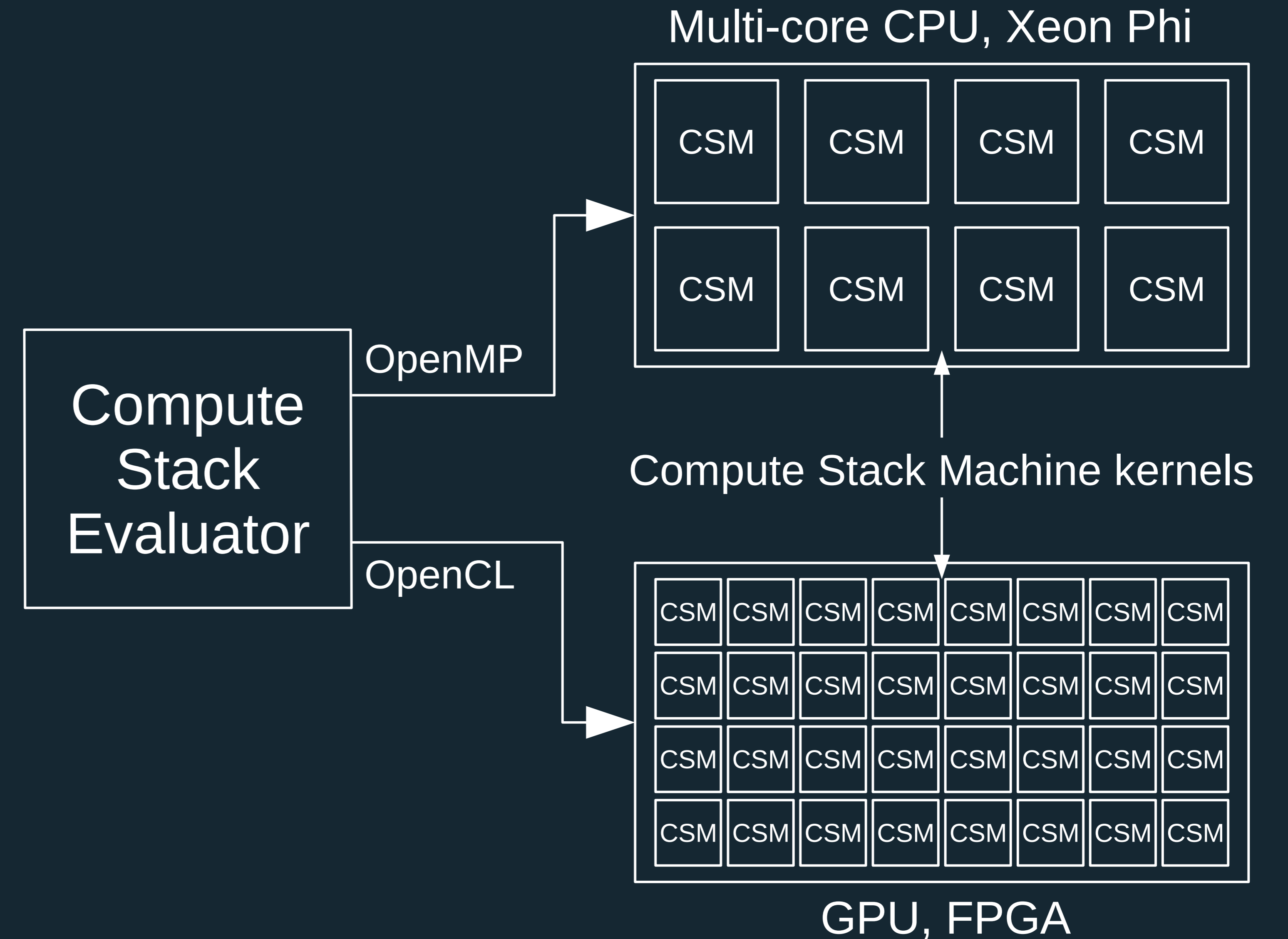


What can be done with OpenCS?

Parallel evaluation of model equations

Systems of equations evaluated using the Compute Stack Evaluator interface:

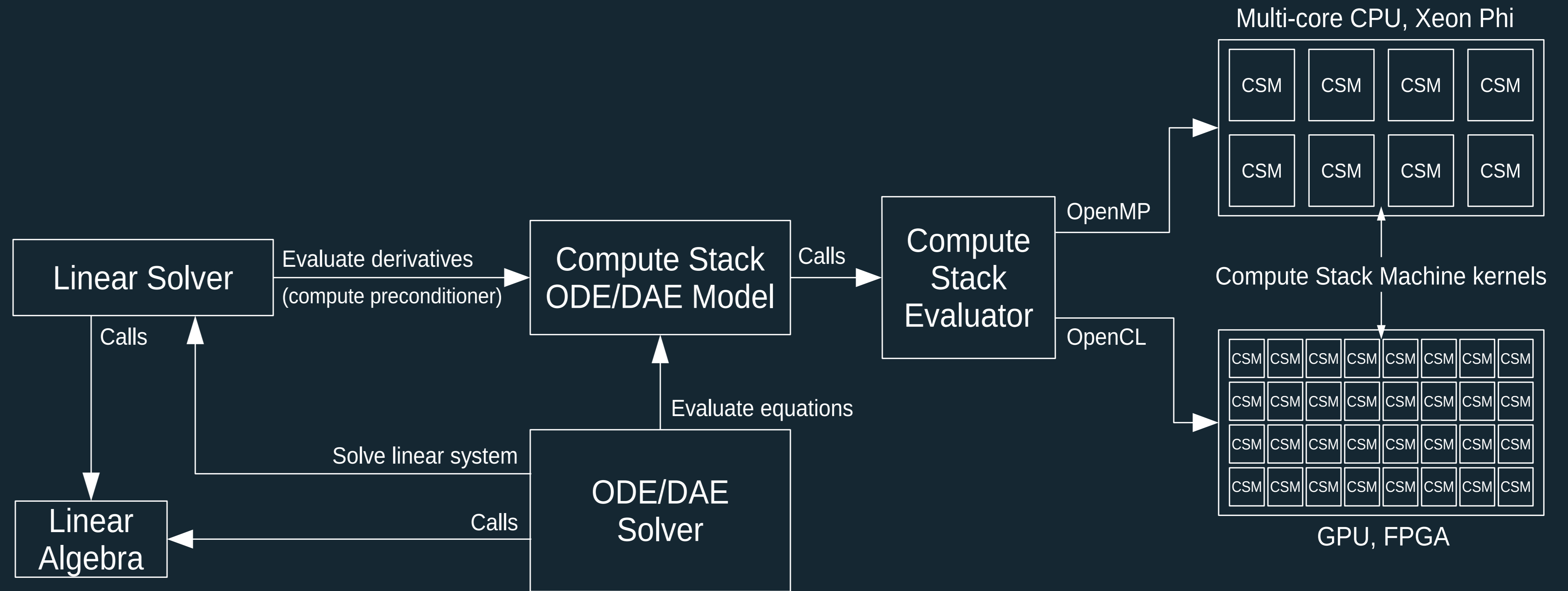
- **OpenMP** for **general purpose processors** (multi-core CPUs, Xeon Phi)
- **OpenCL** for:
 - streaming processors** (GPU, FPGA)
 - heterogeneous systems** (CPU+GPU/FPGA)



What can be done with OpenCS?

Parallel simulation on shared memory systems

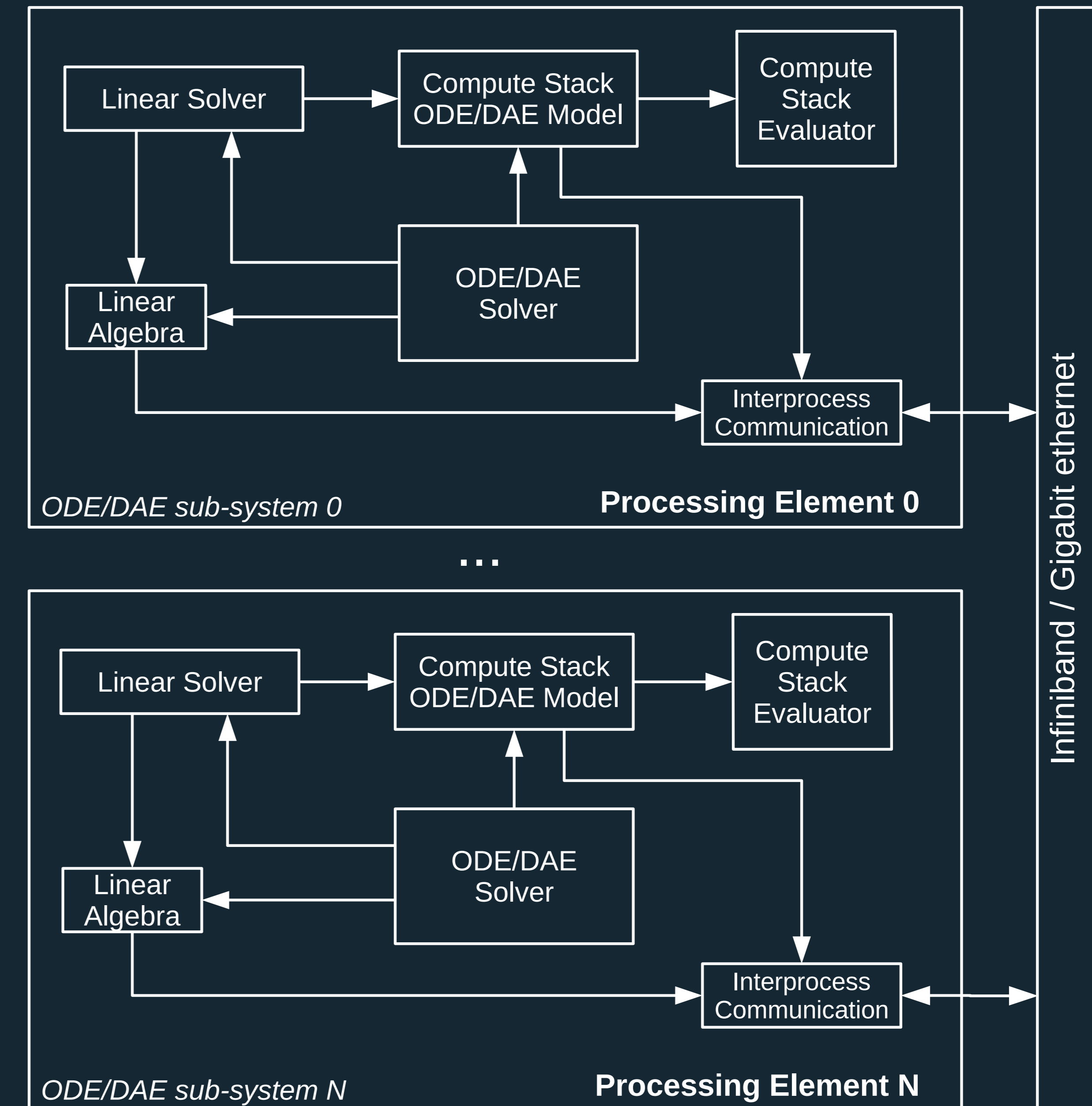
- **Single processing element**
- **Available computing hardware utilised for parallel evaluation of model equations:**
 - Multi-core CPU, Xeon Phi
 - GPU, FPGA
 - Heterogeneous systems i.e. CPU+GPU, CPU+FPGA



What can be done with OpenCS?

Parallel simulation on distributed memory systems

- **Multiple processing elements**
- **Software for simulation on shared memory systems as the main building block**
- **Partitioning using multiple balancing constraints**
- **Every processing element:**
 - Integrates one ODE/DAE sub-system in time
 - Performs an inter-process data exchange



OpenCS benefits

- A **single software** for numerical solution of **any ODE/DAE system** of **any size** on **all platforms**
- The model specification contains only the **low-level model description** (created from any software)
- The **model specification** stored as **files in a platform-independent binary format**
- **Model equations** specified in a **platform independent** way as **an array of binary data**
- Equations can be **evaluated on** virtually **all computing devices** (including heterogeneous systems)
- Switching to a different computing platform for evaluation of equations as an input parameter

The key OpenCS concepts

- Compute Stack:** The Reverse Polish (postfix) notation expression stack to describe and store in computer memory equations of any type and any size
- Compute Stack Machine:** A stack machine used to evaluate a single equation using LIFO queues
- Compute Stack Evaluator:** An interface for parallel evaluation of systems of equations
- Compute Stack Model:** Data structure that holds the low-level model specification
- Compute Stack Differential Equations Model:** A common interface for ODE/DAE solvers for integration of ODE/DAE systems in time
- Compute Stack Simulator:** Sequential/parallel simulator for general ODE/DAE systems
- Compute Stack Model Builder:** A common interface for creation of ODE/DAE Compute Stack models