PRACE Autumn School 2018 - HPC for Engineering and Chemistry

Report of Contributions

Contribution ID: **0** Type: **Presentation**

An introduction to Finite Element, Boundary Element, and Meshless Methods - with applications in heat transfer and fluid flow

Tuesday, September 25, 2018 8:30 AM (3h 30m)

This course presents the Finite Element Method (FEM), Boundary Element Method (BEM) and Meshless Methods (MEM) within a unified framework of the method of weighted residuals (MWR). The course begins by introducing the MWR and one dimensional applications of all three methods as well as finite difference and finite volume methods. The basic fundamentals of the finite element method are then developed using simple examples in heat transfer. Particular attention is given to the development of the discrete set of algebraic equations, beginning with simple one-dimensional problems, illustrating the principles of automated generation of finite elements via Gauss quadratures and body-fitted coordinates, the loading matrix, and continuing to two- and three-dimensional elements. Once these principles are established, the concept of boundary element methods are then introduced. The relation of the BEM to the Green's function approach for the analytical solution of partial differential equations is presented. The advantage of the BEM in reducing the dimensionality of a problem is demonstrated along with applications to problems with infinite domain boundaries. The boundary element technique is a natural extension of the finite element method, and this becomes greatly appreciated by users. The BEM is developed to 2 and 3D problems, symmetric and non-symmetric solvers iterative solvers are presented along with applications in heat transfer and inverse problems. Finally, meshless methods are developed. Here, the focus is on radial basis function (RBF) based meshless formulation in strong form. The method is simple to grasp, and simple to implement. The power of the method is becoming more appreciated with time. The meshless method has been shown to yield solutions with accuracies comparable to finite element methods employing an extensive number of elements, yet requiring no mesh (or connectivity of nodes). We have used it for structural analysis, fluid flow, heat transfer, environmental transport, and various biomedical applications.

Ref: Darrell W. Pepper (University of Nevada Las Vegas), Alain J. Kassab (University of Central Florida), Eduardo A. Divo (Embry-Riddle Aeronautical University), An introduction to finite element, boundary element, and meshless methods with applications to heat transfer and fluid, American Society of Mechanical Engineers (ASME), New York, New York, USA, 2014.

Presenter: Dr KASSAB, Alain (University of Central Florida, Orlando, Florida)

Contribution ID: **1** Type: **not specified**

Welcome address

Monday, September 24, 2018 8:30 AM (15 minutes)

Presenters: Prof. POVH, Janez (University of Ljubljana, ULFME); Prof. DUHOVNIK, Jože (PRACE MB member for Slovenia)

Contribution ID: **2** Type: **not specified**

Parallel Computing

Monday, September 24, 2018 9:30 AM (1 hour)

This course will treat
- the merits and limits of parallel programming
- different parallel programming models (e.g. task and data parallelism)
- the differences between shared and distributed memory systems

Presenter: Mr VAN LEEUWEN, Caspar (SURFsara)

Contribution ID: **3** Type: **not specified**

OpenMP

Monday, September 24, 2018 11:00 AM (1h 15m)

OpenMP is a widely used standard for parallel programming in C/C++/Fortran on shared memory systems.
This course will introduce some basic parallelization and work sharing constructs available in OpenMP and provides hands-on examples to the participants.
The goal is to teach participants how multithreading can be used for parallel computation and to provide them with a starting point from which they can develop their OpenMP knowledge.

Presenter: Mr VAN LEEUWEN, Caspar (SURFSara)

Contribution ID: **4** Type: **not specified**

Conjugate heat transfer and proper orthogonal decomposition

Tuesday, September 25, 2018 3:00 PM (45 minutes)

Presenter: Prof. KASSAB, Alain (University of Central Florida, Orlando, Florida)

Contribution ID: **5** Type: **not specified**

MPI

Monday, September 24, 2018 1:15 PM (2h 15m)

This course will introduce the basic concepts of MPI. The most commonly used routines for sending, receiving, and aggregating data will be explained using hands-on examples.
The goal is to provide participants with a starting point from which they can develop their MPI knowledge, and/or to provide background knowledge for participants using HPC applications that rely on MPI for their communication.

Presenter: Mr VAN LEEUWEN, Caspar (SURFsara)

Contribution ID: **6** Type: **not specified**

Introduction to OpenFoam

Wednesday, September 26, 2018 10:25 AM (1h 45m)

Presenter: Dr GRM, Aleksander (University of Ljubljana, FPP)

Session Classification: HPC in Engineering

Contribution ID: **7** Type: **not specified**

Hands-on tutorial on solving engineering problems with OpenFoam

Wednesday, September 26, 2018 1:15 PM (1h 45m)

- simpleFoam application to simulate steady-state, turbulent, incompressible flow around the vehicle.
- Solving mixed fluid-dissolution problem

Presenter: Dr GRM, Aleksander (University of Ljubljana)

Session Classification: HPC in Engineering

Contribution ID: **8** Type: **not specified**

Presentation of ELIXIR-SI node (structure, organization, mission, and vision)

Contribution ID: **9** Type: **not specified**

HPC resources and services for life sciences (in Slovenia)

Contribution ID: **10** Type: **not specified**

Multiscale CFD modeling for congential heart disease

Wednesday, September 26, 2018 8:30 AM (45 minutes)

Presenter: KASSAB, Alain (U. Florida)

Session Classification: HPC in Engineering

Contribution ID: **11** Type: **not specified**

Hands-on tutorial on comparative genomics and metagenomics

Contribution ID: **12** Type: **not specified**

Multiscale CFD modeling for left ventricular assist device

Wednesday, September 26, 2018 9:15 AM (45 minutes)

Presenter: Prof. KASSAB, Alain (U. Florida)

Session Classification: HPC in Engineering

Contribution ID: **13** Type: **not specified**

Classical and ab-initio molecular dynamics

Wednesday, September 26, 2018 9:15 AM (45 minutes)

Presenter: Dr MERZEL, Franci (KI)

Session Classification: HPC in Chemistry and Chemical engineering

Contribution ID: **14** Type: **not specified**

Quantum methods

Wednesday, September 26, 2018 8:30 AM (45 minutes)

Presenter: Dr STARE, Jernej (KI)

Session Classification: HPC in Chemistry and Chemical engineering

Contribution ID: **15** Type: **not specified**

QM/MM

Wednesday, September 26, 2018 10:30 AM (30 minutes)

Presenter: Dr HODOŠČEK, Milan (KI)

Session Classification: HPC in Chemistry and Chemical engineering

Contribution ID: **16** Type: **not specified**

Multiscale modeling & simulation

Wednesday, September 26, 2018 11:00 AM (30 minutes)

Presenter: Dr PRAPROTNIK, Matej

Session Classification: HPC in Chemistry and Chemical engineering

Contribution ID: **17** Type: **not specified**

Nanofludics

Tuesday, September 25, 2018 1:15 PM (30 minutes)

Presenter: Dr WALTHER, Jens H.

Contribution ID: **18** Type: **not specified**

Hands-on tutorial on Molecular dynamics

Wednesday, September 26, 2018 11:30 AM (45 minutes)

Presenter: Dr HODOŠČEK, Milan (KI)

Session Classification: HPC in Chemistry and Chemical engineering

Contribution ID: **19** Type: **not specified**

Hands-on tutorial on Molecular dynamics and Computational fluid dynamics for nanofluidics

Tuesday, September 25, 2018 1:45 PM (1 hour)

Presenter: Dr WALTHER, Jens H.

Contribution ID: **20** Type: **not specified**

Hands-on tutorial on Quatum methods (Gaussian, cpmd…)

Wednesday, September 26, 2018 1:15 PM (1h 20m)

Presenter: Dr STARE, Jernej (KI)

Session Classification: HPC in Chemistry and Chemical engineering

Contribution ID: **21** Type: **not specified**

Hands-on tutorial on Espresso++

Wednesday, September 26, 2018 2:50 PM (55 minutes)

Presenter: Dr SABLIĆ, Jurij (KI)

Session Classification: HPC in Chemistry and Chemical engineering