



PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

Track B: Particle Methods - Introduction

PRACE Spring School 2012

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Agenda

- **Introduction to Track A** – 10 min.
- **PART1: Particle methods** – 2h
 - Computational problem and implementation ~ 20 min.
 - First look at the code and execution on Notos ~ 30 min.
 - Parallel Random Number Generation (SPRNG) ~ 30 min.
 - Visualization with VisNow ~ 30 min.
- **Coffee break**
- **PART 2: Load-balancing and migration** – 1.5h
 - Zoltan set-up ~ 15 min.
 - Load-balancing in Zoltan ~ 15 min.
 - Hands-on exercises ~20 min.
 - Migration in Zoltan ~ 15 min.
 - Hands-on exercises ~ 25 min.
- **Lunch break**

Agenda continued

- **PART 3: Exchange of particles – 1.5 h**
 - Computing interactions between particles ~ 45 min
 - Hands-on Zoltan neighbourhood assignment ~ 45 min
- **Coffee break**
- **PART 4: Hybrid parallelization and scalability testing – 1h**
 - Hybrid parallelization and execution on the Blue Gene/P architecture ~ 30 min
 - Scalability testing ~ 30 min

Motivation

- I am developing a scalable software that simulates human cell colonies dynamics
- During my work I have found a lot of great tools that:
 - Speeded up the execution of my code (MPI, OpenMP),
 - Speeded up the development process (SPRNG, Zoltan library),
 - Enabled good scalability (Performance Analysis Tools).
- **Efficient parallel implementation of a particle system code is not hard with the use of available libraries**
- **Simple example presented within this training can become a basis for efficient simulation code**

How it is organized?

- Description of problems and tools - presentations
- Hands-on sessions:
 - Description of the exercises given in a presentation
 - Individual work on Notos system
 - For each of the exercise: 3 fastest students will receive a small gift
 - The solution of each exercise will be delivered in a paper copy 10 min before deadline

How it is organized?

Hands-on exercises:

- Start from existing sources
- Learn and implement most important library calls
- End up with parallel particle simulation code
- Implement hybrid MPI + OpenMP parallelization
- Test scalability of the code

List of exercises

- **Exercise 1:** Random number generation **PART 1**
 - **Exercise 2:** Load-balancing
 - **Exercise 3:** Data migration
 - **Exercise 4:** Exchange of particles **PART 3**
 - **Exercise 5:** Hybrid parallelization (MPI+OpenMP)
 - **Exercise 6:** Scalability testing
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