

# Finite Element-Fictitious Boundary Methods for the Numerical Simulation of Particulate Flows



Stefan Turek, Raphael Münster, Otto Mierka Institut für Angewandte Mathematik, TU Dortmund <u>http://www.mathematik.tu-dortmund.de/LS3</u> <u>http://www.featflow.de</u>



#### **Basic CFD Tool:** FeatFlow



<ul> <li>HPC features:</li> <li>Moderately parallel</li> <li>GPU computing</li> <li>Open source</li> </ul>	Hardware -oriented Numerics	<ul> <li>Numerical features</li> <li>Higher order (Q2P) (semi-) Implicit FD/</li> <li>Semi-(un)structure dynamic adaptive g</li> <li>Fictitious Bounda</li> <li>Newton-Multigrid-ty</li> </ul>	<u>:</u> 1) FEM in space & FEM in time d meshes with rid deformation <b>ry (FBM) methods</b> /pe solvers
<ul> <li>Non-Newtonian flow module:</li> <li>generalized Newtonian model (Power-law, Carreau,)</li> <li>viscoelastic model (Giesekus, FENE, Oldroyd,)</li> </ul>	Multiphase flow mo • $\ell/\ell$ – interfac • $s/\ell$ – interfac • $s/\ell/\ell$ – combin	odule (resolved interfaces): ce capturing (Level Set) ce tracking (FBM) nation of the and she	<ul> <li>Engineering aspects:</li> <li>Geometrical design</li> <li>Modulation strategy</li> <li>Optimization</li> </ul>

Here: FEM-based tools for the accurate simulation of multiphase flow problems, particularly with liquid-(rigid) solid interfaces



#### Liquid–(Rigid) Solid Interfaces



Consider the flow of N solid particles in a fluid with density  $\rho$  and viscosity  $\mu$ . Denote by  $\Omega_f(t)$  the domain occupied by the fluid at time t, by  $\Omega_i(t)$  the domain occupied by the ith-particle at time t and let  $\overline{\Omega} = \overline{\Omega}_f \cup \overline{\Omega}_i$ .



The fluid flow is modelled by the **Navier-Stokes equations**:

$$\rho \left( \frac{\partial u}{\partial t} + u \cdot \nabla u \right) - \nabla \cdot \sigma = f, \quad \nabla \cdot u = 0$$

where  $\sigma$  is the total stress tensor of the fluid phase:

$$\sigma(\mathbf{X},t) = -\mathbf{p}\mathbf{I} + \boldsymbol{\mu}[\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathsf{T}}]$$





The motion of particles can be described by the **Newton-Euler equations**. A particle moves with **a translational velocity**  $U_i$  and **angular velocity**  $\omega_i$  which satisfiy:

$$M_{i}\frac{dU_{i}}{dt} = F_{i} + F_{i}' + (\Delta M_{i})g, \qquad I_{i}\frac{d\omega_{i}}{dt} + \omega_{i} \times (I_{i}\omega_{i}) = T_{i,}$$

- M<sub>i</sub> : mass of the i-th particle (i=1,...,N)
- I<sub>i</sub> : moment of inertia tensor of the i-th particle
- $\Delta M_i$  : mass difference between  $M_i$  and the mass of the fluid
- F<sub>i</sub> : hydrodynamic force acting on the i-th particle
- T<sub>i</sub> : hydrodynamic torque acting on the i-th particle





The position and orientation of the i-th particle are obtained by integrating the **kinematic equations**:

$$\frac{dX_{i}}{dt} = U_{i}, \ \frac{d\theta_{i}}{dt} = \omega_{i}, \ \frac{d\omega_{i}}{dt} = I_{i}^{-1}T_{i}$$

which can be done numerically by an explicit Euler scheme:

$$X_{i}^{n+1} = X_{i}^{n} + \Delta t U_{i}^{n} \quad \omega_{I}^{n+1} = \omega_{I}^{n} + \Delta t \left(I_{i}^{-1}T_{i}^{n}\right) \quad \theta_{I}^{n+1} = \theta_{I}^{n} + \Delta t \omega_{I}^{n}$$

# **Boundary Conditions**

We apply the velocity u(X) as no-slip boundary condition at the interface  $\partial \Omega_i$  between the i-th particle and the fluid, which for  $X \in \Omega_i$  is defined by:

$$u(X) = U_i + \omega_i \times (X - X_i)$$



#### **Numerical Solution Scheme**





#### **Fictitious Boundary Method**



#### **Eulerian Approach:**

- FBM = special case of (scaled) Penalty method
- Objects are represented as a boolean (in/out) function on the mesh
- Complex shapes are possible (**surface triangulation, implicit functions**)
- Use of a fixed mesh possible  $\rightarrow$  only first order accurate
- But: Higher accuracy possible by (local) mesh adaptation techniques



# **Dynamic ALE-Mesh Adaptation**



#### Advantages:

- Constant mesh/data structure  $\rightarrow$  GPU
- Increased resolution in regions of interest ("r-adaptivity")
- Anisotropic 'umbrella' smoother (with snapping/projection) or GDM
- Straightforward usage on general meshes in 2D / 3D

Quality of the method depends on the construction of the monitor function

- Geometrical description (solid body, interface triangulation)
- Field oriented description (steep gradients, fronts)  $\rightarrow$  numerical stabilization



Testing: 3D Rising bubble - hard setup

# **Test: Oscillating Cylinder**



- Measure Drag/Lift Coefficients for a sinusoidally oscillating cylinder
- Compare results for FBM, adapted FBM and adapted FBM + boundary projection/parametrization



Nodes concentrated near liquid-solid interface

Nodes projected and parametrized on boundary plus concentration of nodes near boundary



#### **Oscillating Cylinder Results**



Drag Coefficient C<sub>d</sub> for Classic FBM, FBM+adapt, FBM+param+adapt





# **Oscillating Cylinder Results**





# (Passive) Microswimmer







#### **Sedimentation**







#### Viscous Liquid Jets

J. M. Nóbrega et al.: The phenomenon of jet buckling: Experimental and numerical predictions



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# How to calculate the hydrodynamic forces???



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#### **Hydrodynamic Forces**



#### Hydrodynamic force and torque acting on the i-th particle

$$F_{i} = -\int_{\partial\Omega_{i}} \sigma \cdot n_{i} d\Gamma_{i}, \quad T_{i} = -\int_{\partial\Omega_{i}} (X - X_{i}) \times (\sigma \cdot n_{i}) d\Gamma$$

#### **Force Calculation with Fictitious Boundary Method**

#### **Problems: The FBM can only decide:**

- `INSIDE`(1) and `OUTSIDE`(0)
- No description of the surface



# Alternative: Replace the surface integral by a volume integral





Define an *indicator function*  $\alpha_i$ :

$$\alpha_{i}(X) = \begin{cases} 1 & \text{for } X \in \Omega_{i} \\ 0 & \text{for } X \in \Omega_{f} \end{cases}$$

**Remark:** The gradient of  $\alpha_i$  is zero everywhere except at the surface of the i-th Particle and approximates the normal vector (in a weak sense), allowing us to write:

$$F_{i} = -\int_{\Omega_{\tau}} \sigma \cdot \nabla \alpha_{i} d\Omega , \quad T_{i} = -\int_{\Omega_{\tau}} (X - X_{i}) \times (\sigma \cdot \nabla \alpha_{i}) d\Omega$$



#### **Numerical Force Evaluation (II)**



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# Large-scale FBM-Simulations



#### Integration over $\Omega_T$ too expensive:

- Gradient is non-zero on  $\partial \Omega_i$
- Information available from FBM
- Evaluate boundary cells only
- Visit each cell only once

$$= -\sum_{\mathbf{I} \in \mathbf{Ih}, \mathbf{\Omega}} \int_{\Omega} \sigma_{\mathbf{h}} \cdot \nabla \alpha_{\mathbf{h}j} d\Omega ,$$

$$- \sum_{T_{i} \in T_{h,i}} \int_{\Omega_{T}} (X - X_{i}) \times (\sigma_{h} \cdot \nabla \alpha_{h,i}) d\Omega$$

 $\alpha_{h,i}(x)$  : finite element interpolant of  $\alpha(x)$ T<sub>h,i</sub> : elements intersected by i-th particle

#### **Contact/Collision Modelling**



- **Contact determination** for rigid bodies A and B:
  - $\rightarrow$  Distance d(A,B)
  - → Relative velocity  $v_{AB} = (v_A + \omega_A \times r_A (v_B + \omega_B \times r_B))$
  - $\rightarrow$  Collision normal N = (X<sub>A</sub> (t) X<sub>B</sub> (t))
  - $\rightarrow$  Relative normal velocity N · (v<sub>A</sub> +  $\omega_A \times r_A (v_B + \omega_B \times r_B))$
- Contact force calculation realized as a three step process
  - → Broad phase
  - → Narrow phase
  - → Contact/Collision force calculation

Several single, resp., multibody collision models are realized and tested, but.....





# How to validate???



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#### **Benchmarking and Validation (I)**



#### Free fall of particles:

- Terminal velocity
- Different physical parameters
- Different geometrical parameters



*Münster, R.; Mierka, O.; Turek, S.:* Finite Element fictitious boundary methods (FEM-FBM) for 3D particulate flow, IJNMF, 2011



Source: Glowinski et al. 2001

### **Benchmarking and Validation (II)**

Settling of a sphere towards a plane wall:

- Sedimentation Velocity
- Particle trajectory
- Kinetic Energy
- Different Reynolds numbers



#### Setup

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Computational mesh:

- 1.075.200 vertices
- 622.592 hexahedral cells

• Q2/P1:

TU

→ 50.429.952 DoFs



#### 0.894 0.947 0.950 0.953

 $u_{max}/u_{\infty}$ 

exp

11.6 0.959 0.951 0.947 0.955 31.9 Tab. 1 Comparison of the  $u_{max}/u_{\infty}$  ratios between the FEM-FBM, ten Cate's simulation and ten Cate's

experiment

Re

1.5

4.1

 $u_{max}/u_{\infty}$ 

0.945

0.955

0.953

# Sedimentation Benchmark (I)

#### **Observations**

- Velocity profiles compare well to ten Cate's data
- Maximum velocity close to experiment
- Flow features are accurately resolved •





 $u_{max}/u_{\infty}$ 

ten Cate

0.955





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#### **Sedimentation Benchmark (II)**





Source: 13th Workshop on Two-Phase Flow Predictions 2012 Acknowledgements: Ernst, M., Dietzel, M., Sommerfeld, M.



#### **Sedimentation Benchmark (III)**



#### FEM-Multigrid Framework

- Increasing the mesh resolution produces more accurate results Test performed at different mesh levels
  - Maximum velocity is approximated better
  - Shape of the velocity curve matches better







# Now let's get it "colorful"...



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#### **Some More Complex Examples**













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# (More) Complex Geometry Examples





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#### Fluidized Bed Example









# ...and finally some applications of FBM...



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## **Example: (Active)** Microswimmer

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Application to microswimmers (published: Nature Comm.)

- Exp.: Cooperation with AG Fischer (MPI IS Stuttgart)
- Analysis with respect to shear thickening/thinning
- Use of grid deformation to resolve *s/l* interface





#### **Example: Screw Extruder (I)**



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- Numerical simulation of (partially filled) (twin)screw extruders
- *Non-Newtonian rheological* models (shear & temperature dependent) with *non-isothermal* conditions (cooling from outside, heat production)
- Analysis of the influence of local characteristics on the global product quality, prediction of hotspots and maximum shear rates
- Optimization of torque acting on the screws, energy consumption





#### **Example: Screw Extruder (III)**



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#### **Example: Virtual Wind Tunnel (I)**

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- Numerical simulation of complex geometries
- Use of a regular semi-unstructured preadapted mesh
- Resolution of small scale details by local mesh adaptation



#### **Influence of Mesh Adaptation (II)**

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Car representation by the computational mesh



- Details may be lost without adaptation
- Better resolution with the same number of DOFs
- Mesh adaptation saves at least one refinement level



#### **Example: Fluid Prilling&Encapsulation**

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- Numerical simulation of *micro-fluidic drug encapsulation ("monodisperse compound droplets")*
- Polymeric "bio-degradable" outer fluid with generalized Newtonian behaviour
- Optimization w.r.t. boundary conditions, flow rates, droplet size, geometry



#### **Extensions & Future Activities**



#### Fluidics

- Viscoelastic fluids
- Multiphase problems
  - → Liquid-Liquid-Solid
  - → Melting/Solidification

#### Hardware-Oriented Numerics

- Improve parallel efficiency of collision detection and force computation on GPU
- Dynamic grid adaptation with snapping

#### More communication between the scientific communities is required!

#### Benchmarking

- 1 "complex" object
- "Many" (=2) objects!





# Backup slides ...



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#### **Complex Rigid Bodies (I)**



Geometric representation:
 → Surface triangulation







#### **Complex Rigid Bodies (II)**



#### Moment of Inertia Tensor:

- Can be calculated in a preprocessing step using FEM software
- Moment of inertia tensor changes as the body moves and rotates
  - → Transform the moment of inertia tensor by the transformation matrix of the rigid body

$$\begin{bmatrix} I_{xx} & 0 & 0 \\ 0 & I_{yy} & 0 \\ 0 & 0 & I_{zz} \end{bmatrix} \qquad \begin{bmatrix} I_{xx} & -I_{xy} & -I_{xz} \\ -I_{xy} & I_{yy} & -I_{yz} \\ -I_{xz} & -I_{yz} & I_{zz} \end{bmatrix}$$

$$I_{xx} = \int_{P} (y^{2} + z^{2})\rho(x, y, z)dP \qquad I_{xy} = \int_{P} xy \cdot \rho(x, y, z)dP$$

$$I_{yy} = \int_{P} (x^{2} + z^{2})\rho(x, y, z)dP \qquad I_{xz} = \int_{P} xz \cdot \rho(x, y, z)dP$$

$$I_{zz} = \int_{P} (x^{2} + y^{2})\rho(x, y, z)dP \qquad I_{yz} = \int_{P} yz \cdot \rho(x, y, z)dP$$

$$Transformation of I: \qquad I_{w} = M_{Iw} \cdot I \cdot M_{Iw}^{T}$$

#### **Spatial Partitioning/Uniform Grids**



- Cell size relates to radius of (bounding) sphere
- Only objects in neighbouring cells are candidates for collision .
- Multiple grid levels for objects of different size
- Efficient storage by using a hash mapping



#### **Collision Pipeline on the GPU (I)**



Collision Detection

- Domain is covered by a uniform grid or Aspatial hash
  - $\rightarrow$  use cell size equal to particle diameter
- Sort particles with GPU Radix sort by grid cell index
  - $\rightarrow$  Need to check only neighbouring cells for collisions
  - $\rightarrow$  Sorting leads to cache efficient grid traversal



#### **Collision Pipeline on the GPU (II)**

Collision forces

- Use a DEM approach that can be easily evaluated in parallel
- Consider only the 3x3x3 neighbouring cells for each particle



Can be extended to rigid bodiesDetails: GPU Gems 3 (Takahiro Harada)



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#### **Multi-Body Collision Model (III)**

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Sequential Impulses

- Apply pairwise impulses iteratively

Normal impulse  $P_n = \max\left(\frac{-\Delta \overline{\mathbf{v}} \cdot \mathbf{n}}{k_n}, 0\right)$ 

Tangential (frictional) impulse



- Terminate when:
  - Impulses become small
  - Iteration limit is reached

$$P_t = \text{clamp}(\frac{-\Delta \overline{\mathbf{v}} \cdot \mathbf{t}}{k_t}, -\mu P_n, \mu P_n)$$

$$k_t = \frac{1}{m_1} + \frac{1}{m_2} + \left[ I_1^{-1} \left( \mathbf{r}_1 \times \mathbf{t} \right) \times \mathbf{r}_1 + I_2^{-1} \left( \mathbf{r}_2 \times \mathbf{t} \right) \times \mathbf{r}_2 \right] \cdot \mathbf{t}$$

Details: Guendelman, Nonconvex rigid bodies with stacking

#### **Multi-Body Collision Model (II)**



$$\begin{split} & w = Ax + b, \quad w, x, b \in R^{n}, A \in R^{n \times n}, w, x, b \ge 0\\ & \left(w_{1}x_{1}, \dots, w_{n}x_{n}\right) = \left(0, \dots, 0\right)\\ & A_{1k} = \delta_{i_{1}i_{k}} n_{1}^{T} \left(\frac{1}{m_{i_{k}}} 1_{3 \times 3} - r_{1i_{1}}^{\times} I_{i_{k}}^{-1} r_{ki_{k}}^{\times}\right) n_{k} - \delta_{i_{1}j_{k}} n_{1}^{T} \left(\frac{1}{m_{j_{k}}} 1_{3 \times 3} - r_{1i_{1}}^{\times} I_{j_{k}}^{-1} r_{kj_{k}}^{\times}\right) n_{k}\\ & - \delta_{j_{1}i_{k}} n_{1}^{T} \left(\frac{1}{m_{i_{k}}} 1_{3 \times 3} - r_{j_{1}}^{\times} I_{i_{k}}^{-1} r_{ki_{k}}^{\times}\right) n_{k} + \delta_{j_{1}j_{k}} n_{1}^{T} \left(\frac{1}{m_{j_{k}}} 1_{3 \times 3} - r_{j_{1}}^{\times} I_{j_{k}}^{-1} r_{kj_{k}}^{\times}\right) n_{k} \end{split}$$

This LCP can be solved with efficient iterative methods like the projected Gauss-Seidel solver (PGS).



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#### **Grid Deformation Method**

**Idea** : construct transformation  $\phi$ ,  $x = \phi(\xi, t)$ with det  $\nabla \phi = f$  $\implies$  local mesh area  $\approx f$ 

**1.** Compute monitor function  $f(x,t) > 0, f \in C^1$ and  $\int_{\Omega} f^{-1}(x,t) dx = |\Omega|, \quad \forall t \in [0,1]$ 

2. Solve 
$$(t \in [0,1])$$
  
 $\Delta v(\xi, t) = -\frac{\partial}{\partial t} \left( \frac{1}{f(\xi, t)} \right), \quad \frac{\partial v}{\partial n} \Big|_{\partial \Omega} = 0$ 

3. Solve the ODE system

$$\frac{\partial}{\partial t}\phi\left(\xi,t\right) = f\left(\phi\left(\xi,t\right),t\right)\nabla v\left(\phi\left(\xi,t\right),t\right)$$

new grid points:  $x_i = \phi(\xi_i, 1)$ 

Grid deformation preserves the (local) logical structure



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#### **Multi-Body Collision Model (II)**



$$\begin{split} & w = Ax + b, \quad w, x, b \in R^{n}, A \in R^{n \times n}, w, x, b \ge 0 \\ & (w_{1}x_{1}, ..., w_{n}x_{n}) = (0, ..., 0) \end{split}$$
$$A | k = \delta_{ijk}n |^{T} \left(\frac{1}{m_{ik}} 1_{3 \times 3} - r_{ij} | i_{ik} r_{kk} \right) n_{k} - \delta_{ijk}n |^{T} \left(\frac{1}{m_{jk}} 1_{3 \times 3} - r_{ij} | i_{jk} r_{kj} \right) n_{k} - \delta_{ijk}n |^{T} \left(\frac{1}{m_{jk}} 1_{3 \times 3} - r_{ij} | i_{jk} r_{kj} \right) n_{k}$$
$$- \delta_{jik}n |^{T} \left(\frac{1}{m_{ik}} 1_{3 \times 3} - r_{ij} | i_{k} r_{kk} \right) n_{k} + \delta_{jijk}n |^{T} \left(\frac{1}{m_{jk}} 1_{3 \times 3} - r_{ij} | i_{jk} r_{kj} \right) n_{k}$$

This LCP can be solved with efficient iterative methods like the projected Gauss-Seidel solver (PGS).



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#### **Efficient FBM Calculation**



#### Efficient large-scale FBM

For *n* particles and *m* dofs a naive calculation of the inside/outside function on the grid has a complexity of  $O(n \cdot m)$ 

Neccessary only if the grid data structure does not have links between the cell index and the geometric location of the cell

#### Exploit temporal coherency

- The particle trajectory is relatively smooth
- Change in position between timesteps is small
   **FBM Update Strategy**
- $\rightarrow$  Store the cells intersected by a particle in t<sub>n</sub>
- $\rightarrow$  Start neighbour search from these cells in t<sub>n+1</sub>
- $\rightarrow$  While cell is in object and not visited:
  - → Store cell, mark as visited
  - → Search next neighbour
- $\rightarrow$  Number of cells visited is a constant:
  - $\rightarrow$  Update complexity: O(n)

Alternative:

#### **Hierarchical Uniform Hash Grids**





#### **Examples**

- Flows with complex geometries
- Fluidized bed
- Particulate flow demonstrating incompressibility
- GPU sedimentation example
- Numerical results and benchmark test cases
- Comparison of results with other groups





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#### **Microswimmer Example**









Compared to the classic FBM approach the force curve is much smoother with grid adaptation



# **Microswimmer Example**











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# **Driven Cavity with Particles**







#### **Contact/Collision Modelling**





- $\rightarrow$  Distance d(A,B)
- → Relative velocity  $v_{AB} = (v_A + \omega_A \times r_A (v_B + \omega_B \times r_B))$
- $\rightarrow$  Collision normal N = (X<sub>A</sub> (t) X<sub>B</sub> (t))
- $\rightarrow$  Relative normal velocity N · (v<sub>A</sub> +  $\omega_A \times r_A (v_B + \omega_B \times r_B))$
- distinguishes three cases of how bodies move relative to each other:
  - $\rightarrow$  Colliding contact : N · v<sub>AB</sub> < 0
  - $\rightarrow$  Separation : N · v<sub>AB</sub> > 0

$$\rightarrow$$
 Touching contact : N · v<sub>AB</sub> = 0



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# **Contact Force Calculation**

- Contact force calculation realized as a three step process
  - → Broad phase
  - → Narrow phase
  - → Contact/Collision force calculation
- Worst case complexity for collision detection is O(n<sup>2</sup>)
  - → Computing contact information is expensive
  - → Reduce number of expensive tests → Broad Phase
- Broad phase
  - $\rightarrow$  Simple rejection tests exclude pairs that cannot intersect
  - → Use hierarchical spatial partitioning
- Narrow phase
  - → Uses Broadphase output
  - $\rightarrow$  Calculates data neccessary for collision force calculation
  - Several single, resp., multibody collision models are realized and tested, but.....







#### **Single Body Collision Model**

For a single pair of colliding bodies we compute the impulse f that causes the velocities of the bodies to change:

$$f = \frac{-(1 + \epsilon)(n_1(v_1 - v_2) + \omega_1(r_{11} \times n_1) - \omega_2(r_{12} \times n_1))}{m_1^{-1} + m_2^{-1} + (r_{11} \times n_1)^T I_1^{-1}(r_{11} \times n_1) + (r_{12} \times n_1)^T I_2^{-1}(r_{12} \times n_1)}$$

Using the impulse f, the change in linear and angular velocity can be calculated:

$$v_{1}(t + \Delta t) = v_{1}(t) + \frac{fn_{1}}{m_{1}}, \omega_{1}(t + \Delta t) = \omega_{1}(t) + l_{1}^{-1}(r_{11} \times fn_{1})$$
$$v_{2}(t + \Delta t) = v_{2}(t) - \frac{fn_{1}}{m_{2}}, \omega_{2}(t + \Delta t) = \omega_{2}(t) - l_{2}^{-1}(r_{12} \times fn_{1})$$



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#### **Multi-Body Collision Model**



In the case of **multiple colliding bodies** with *K* contact points the impulses influence each other. Hence, they are combined into a system of equations that involves the following matrices and vectors:

- N: matrix of contact normals
- C: matrix of contact conditions
- M: rigid body mass matrix
- f: vector of contact forces (f<sub>i</sub>≥0)
- f<sup>ext</sup>: vector of external forces(gravity, etc.)

$$\frac{N^{\mathsf{T}}C^{\mathsf{T}}M^{-1}CN}{A} \cdot \frac{\Delta tf^{t+\Delta t}}{x} + \frac{N^{\mathsf{T}}C^{\mathsf{T}}\left(u^{t} + \Delta tM^{-1} + f^{ext}\right)}{b} \ge 0, f \ge 0$$

A problem of this form is called a Linear Complementarity Problem (LCP) which can be solved with efficient iterative methods like the **Projected Gauss-Seidel solver (PGS)**.

Kenny Erleben, Stable, Robust, and Versatile Multibody Dynamics Animation



# **DGS Configuration**





