

Solving Partial Differential equations on adaptive point clouds

A part of an open source meshless project **Medusa** https://gitlab.com/e62Lab/medusa http://e6.ijs.si/medusa/

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Basic info

Jožef Stefan Institute

Leading Slovenian research organization

The Jožef Stefan Institute is named after the distinguished 19th century physicist Jožef Stefan, most famous for his work on the Stefan-Boltzmann law of black-body radiation and Stefan's problems (study of ice growth)







1200 employees Revenue approximately - 85 M€ 60 % national programme – 10 % applied research - 10 % international projects – 20 % industrial contracts 430+ ongoing national and international projects



JSI HQ in Ljubljana, Jamova cesta 39

IJS Reactor Center Podgorica



Jožef Stefan Institute

There are three main research branches at JSI

Physics:

- Theoretical Physics
- Low and Medium Energy Physics
- Thin Films and Surfaces,
- Surface Engineering and Optoelectronics,
- Condensed Matter Physics,
- Complex Matter, Reactor Physics,
- Experimental Particle Physics

Electronics and Information Technologies

- Automation,
- Bio-cybernetics and Robotics,
- Systems and Control,
- Artificial Intelligence,
- Open Computer Systems and Networks,
- Communication Systems (P-Lab)
- Computer Systems,
- Knowledge Technologies,
- Intelligent Systems

Chemistry and Biochemistry:

- Biochemistry and Molecular Biology
- Molecular and Biomedical Sciences,
- Biotechnology,
- Inorganic Chemistry and Technology,
- Electronic Ceramics, Engineering Ceramics,
- Nanostructured Materials,
- Synthesis of Materials,
- Advanced Materials
- Environmental Sciences







Parallel and distributed systems laboratory

One of three Laboratories from Communication Systems departmen

Team: 6 full time researchers (3 PhD students) :: 2 part time researches :: 1 technician :: 7 MSc students



Interested in: Scientific computing.

Active projects



Inertial effects on fluid flow in complex porous media (NCN-ARRS)



Advanced concept of efficient use of transformers leveraging the DTR technology (Applied)

Cryptographically secure random number generator(Applied)

Downscaling

meteorological

terrain(applied)



Advanced modelling of radio channels using meshless methods (ARRS)



intelligence is coaching you (ARRS)



Graph Theory and Combinatorial Scientific Computing (OTKA-ARRS)

ctenophore blooms (ARRS)



Past climate change and glaciation at the Alps-Dinarides junction(ARRS)



DiTeR: Dynamic thermal line rating of power lines (Applied)



Forecasting tap changer regulatory maintenance with advanced analytics variables over complex (Applied)







of an invasive



Meshless numerical methods for solving PDEs



efficient implementation of numerical solution procedure

Differential operator approximation

The main idea behind meshless method is the approximation of differential operators over the local cluster of nodes, in many cases simply *n* closest nodes

Differential operator is approximated as

$$(\mathcal{L}u)(x_i) \approx \sum_{x_j \in N(x_i)} w_j^i u(x_j)$$

Imposing exactness for a certain set of basis functions, e.g. monomials, MQs, Gaussians, etc., results in a system

$$\begin{bmatrix} \varphi(\|x_{j_1} - x_{j_1}\|) & \cdots & \varphi(\|x_{j_{n_i}} - x_{j_1}\|) \\ \vdots & \ddots & \vdots \\ \varphi(\|x_{j_1} - x_{j_{n_i}}\|) & \cdots & \varphi(\|x_{j_{n_i}} - x_{j_{n_i}}\|) \end{bmatrix} \begin{bmatrix} w_{j_1}^i \\ \vdots \\ w_{j_{n_i}}^i \end{bmatrix} = \begin{bmatrix} (\mathcal{L}\varphi_{j_1})(x_i) \\ \vdots \\ (\mathcal{L}\varphi_{j_{n_i}})(x_i) \end{bmatrix}$$

That can be subjected to additional weighting (W), when working with more nodes in support than basis functions (n>m) [1]

To enforce consistency of the approximation system can be augmented with monomials up to a certain order

$$\begin{bmatrix} A & P \\ P^{\mathsf{T}} & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{w} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \boldsymbol{\ell}_{\varphi} \\ \boldsymbol{\ell}_{p} \end{bmatrix} \qquad P = \begin{bmatrix} p_{1}(\boldsymbol{x}_{1}) & \cdots & p_{s}(\boldsymbol{x}_{1}) \\ \vdots & \ddots & \vdots \\ p_{1}(\boldsymbol{x}_{n}) & \cdots & p_{s}(\boldsymbol{x}_{n}) \end{bmatrix}, \quad \boldsymbol{\ell}_{p} = \begin{bmatrix} (\mathcal{L}p_{1})|_{\boldsymbol{x}=\boldsymbol{x}^{*}} \\ \vdots \\ (\mathcal{L}p_{s})|_{\boldsymbol{x}=\boldsymbol{x}^{*}} \end{bmatrix}$$



[1] http://e6.ijs.si/medusa/wiki/index.php/Computation_of_shape_functions

Differential operator approximation

Several strong form methods that can be described with this approach

Finite Differences Method	\longrightarrow	n=3, W(p)=1, b={1, x, x2} on regular nodes
Local Radial Basis Function Collocation Method Šarler, B. (2007): From global to local radial basis function collocatio method for transport phenomena, Advances in Meshfree Technique Springer, Berlin, pp. 257-282.	on Əs,	n, W(p)=1, b={sqrt(1+(p/c)2)}, m=n
Finite pointset method S Tiwari, J Kuhnert - Meshfree methods for partial differential equation 2003 - Springer	ons,	n=20-50, W(p)=exp(-(p/s)2), b={1, x, x^2,}
Diffuse Approximate Method Diffuse approximation method for solving natural convection in porou media, C Prax, H Sadat, P Salagnac - Transport in Porous Media, 19 Springer	→ us 996 -	n=13, W(p)=exp(-(p/s)2), b ={1, x, y, x^2, y^2, xy}
Radial basis function generated finite differences (RBF-FD) Accuracy of radial basis function interpolation and derivative approxi on 1-D infinite grids, B Fornberg, N. Flyer - Advances in Computation Mathematics, 2005 – Springer	imations nal	n=12, basis = r^3, augmentation ={1, x, y, x^2, y^2, xy}

... and many more

. .

More details on differential operator approximation such as complexity analysis, ghost nodes, boundary conditions, implementation notes, stability, ... can be found at out discussion wiki page -- http://e6.ijs.si/medusa/wiki/index.php/Medusa

Discretization of the domain

Uscretization of the domain

It is generally accepted that quasi-uniformly-spaced node sets improve the stability of meshless methods

Holger Wendland. Scattered data approximation. Number 17 in Cambridge Monographs on Applied and Computational Mathematics. Cambridge University Press, 2004

The most basic way to generate node sets is to employ existing tools and algorithms for mesh generation, use the generated nodes and simply discard the connectivity relations

(G.-R. Liu, Mesh free methods: moving beyond the finite element method, CRC press, 2002)

- Conceptually flawed
- Expensive
- Inappropriate for meshless

A common iterative approach is to position nodes by simulating free charged particles, obtaining so-called minimal energy nodes, Other iterative methods include bubble simulation, Voronoi relaxation or a combination of both. [17, 24, 1] (*D. P. Hardin and E. B. Saff, Discretizing manifolds via minimum energy points, Notices of the AMS, 51 (2004), pp. 1186-1194 Y. Liu, Y. Nie, W. Zhang, and L. Wang, Node placement method by bubble simulation and its application, Computer Modeling in Engineering and Sciences (CMES), 55 (2010),*

Y. Liu, Y. Nie, W. Zhang, and L. Wang, Node placement method by bubble simulation and its application, Computer Modeling in Engineering and Sciences(CMES), 55 (2010), p. 89)

- Iterative methods are computationally expensive and require an initial distribution
- can be used as a post processing

Advancing front methods, which usually begin at the boundary and advance towards the domain interior, filling it in the process. *(R. Lohner and E. Onate , A general advancing front technique for filling space with arbitrary objects, Int. J. Numer. Methods Eng., 61 (2004), pp. 1977)*

• Often limited to 2D

Circle or sphere packing methods

(X.-Y. Li, S.-H. Teng, and A. Ungor, Point placement for meshless methods using sphere packing and advancing front methods, in ICCES'00, Los Angeles, CA, Citeseer, 2000.)

- Expensive
- Good quality of nodal distribution

Poisson Disk sampling based algorithms (also advancing front type node generation)

(R. L. Cook, Stochastic sampling in computer graphics, ACM Trans. Graphics, 5 (1986), pp. 51

V. Shankar, R. M. Kirby, and A. L. Fogelson, Robust node generation for meshfree discretizations on irregular domains and surfaces, SIAM J. Sci. Comput., 40 (2018), pp. 2584 Slak J., Kosec G., On Generation of Node Distributions for Meshless PDE Discretizations, SIAM Journal on Scientific Computing, 41(5))

- Computationally effective
- Dimension independent
- Good quality of nodal distribution

Meshless node generation

vleshless node generation

Dimension independent Poisson disc sampling based node generation algorithm supporting spatially variable density distribution

- Local regularity with minimal spacing guaranteed
- Spatially variable density
- Scalable

- Compatible with irregular domains
- Dimension independent



Extension to parametric surfaces and CAD geometry

Extension to parametric surfaces and CAD geometry







Node sets generated by NURBS-DIVG on a CAD Utah Teapot (left) and a CAD model of tiger (right). The Utah Teapot model is made of 32 patches and has 7031 nodes; the tiger has 124 patches and 4753 boundary nodes.

CAD models typically consist of multiple non-overlapping and abutting NURBS surface patches. A NURBS patch meets another NURBS patch at a NURBS curve (the boundary curves of the respective patches)





We can change the order of the method by varying order of augmenting monomials (*p*-adaptivity/refinement)

• Higher order method requires bigger stencil $-n = 2\binom{m+d}{d}$

m	d = 1	d = 2	d = 3	
2	6	12	20	
4	10	30	70	
6	14	56	168	
8	18	90	330	

We can control local internodal distance via density function in DIVG node positioning algorithm (*h*-adaptivity/refinement)

h – adaptivity/refinement is inherently included in the meshless methods





Adaptive solution procedure

- Solve governing PDE with given node and order distribution.
- Estimate error
- Mark nodes for refinement/derefinement
- Recompute with new setup
- repeat



The modified Texas Three-Fold marking strategy

Each node is tested for refinement action based on error indicator (or actual error or any other quantity we would like to consider)





Example of 4 step *h*-refinement of a simple test function approximation with nodal density increase factor *f*



IMEX Error indicator

INLEX HEROFINGIC

Consider a problem of type

 $\mathcal{L}u = f_{RHS}.$

The \underline{IM} plicit- \underline{EX} plicit error indicator:

- 1. Obtain implicit solution $u^{(im)}$ to governing problem using low-order approximations of \mathcal{L} , i.e. $\mathcal{L}_{(im)}^{(lo)}$.
- 2. Obtain high-order approximations or explicit operators \mathcal{L} , i.e. $\mathcal{L}_{(ex)}^{(hi)}$
- 3. Apply $\mathcal{L}_{(ex)}^{(hi)}$ to $u^{(im)}$ and obtain $f_{(ex)}$ the process
- 4. Compare f_{RHS} and $f_{(ex)}$

$$\nabla^2 u(\mathbf{x}) = 2ae^{-a||\mathbf{x}-\mathbf{x}_s||^2} (2a ||\mathbf{x}-\mathbf{x}_s|| - d) \quad \text{in } \Omega,$$

$$u(\mathbf{x}) = e^{-a||\mathbf{x}-\mathbf{x}_s||^2} \qquad \text{on } \Gamma_d,$$

$$\nabla u(\mathbf{x}) = -2a(\mathbf{x}-\mathbf{x}_s)e^{-a||\mathbf{x}-\mathbf{x}_s||^2} \qquad \text{on } \Gamma_n,$$



1.0

High order solution of Poisson's problem

2h order solution of Poisson's provieu



• Adaptive solution of Poisson's problem

numerical solution

x

1.0

1.0 -

0.8

0.6

0.4

0.2

0.0

0.0 0.2 0.4 0.6 0.8

 \succ

Poisson problem with exponentially strong source in the domain

$$\begin{aligned} \nabla^2 u(\mathbf{x}) &= 2ae^{-a\|\mathbf{x}-\mathbf{x}_s\|^2}(2a\|\mathbf{x}-\mathbf{x}_s\|-d) & \text{ in } \Omega, \\ u(\mathbf{x}) &= e^{-a\|\mathbf{x}-\mathbf{x}_s\|^2} & \text{ on } \Gamma_d, \\ \nabla u(\mathbf{x}) &= -2a(\mathbf{x}-\mathbf{x}_s)e^{-a\|\mathbf{x}-\mathbf{x}_s\|^2} & \text{ on } \Gamma_n \end{aligned}$$

Setup

- RBF-FD
- PHS order k = 3
- Monomial augmentation with $m \in \{2, 4, 6, 8\}$
- IMEX with monomials $m \in \{4, 6, 8, 10\}$





Adaptive fretting fatigue simulation



smallest internodal distance is 2^{17} times smaller than the initial one

Consideration of irregular 3D domains

Consideration of irregular 3D domains



Elastic deformation of a 3D gear object that is subjected to the external torque resulting in the tangential traction on axis, while the gear teeth are blocked.

$$\begin{split} \frac{E}{2\left(\nu+1\right)} \left(\nabla^2 \mathbf{u} + \frac{1}{1-2\nu} \nabla \left(\nabla \cdot \mathbf{u}\right) \right) &= 0\\ \mathbf{u} &= 0, \quad \text{on } \Gamma_{\text{teeth}},\\ \sigma \cdot \mathbf{n} &= 0, \quad \text{on } \Gamma_{\text{free}},\\ \sigma \cdot \mathbf{t} &= t_0 \mathbf{t}, \quad \text{on } \Gamma_{\text{axis}}. \end{split}$$





Non-Newtonian natural convection in randomly generated domain with differentially heated vertical walls and isolated horizontal walls

$$\nabla \cdot \boldsymbol{v} = 0,$$

$$\rho(\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v}) = -\nabla p + \nabla \cdot (\eta \nabla \boldsymbol{v}) - \boldsymbol{g}\rho\beta T_{\Delta},$$

$$\rho c_p(\frac{\partial T}{\partial t} + \boldsymbol{v} \cdot \nabla T) = \nabla \cdot (\lambda \nabla T),$$

$$\eta = \eta_0 \left(\frac{1}{2} \|\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T\|\right)^{\frac{n-1}{2}},$$

Moving boundary problems

Meshless interface tracking for the simulation of dendrite envelope growth including surface reconstruction and h-adaptive cloud points.



Solidification of a binary alloy



Adaptive upwind





Concentration and velocity at different stages of Sn-10%Pb alloy solidification. Last (bottom right) plot stands for fully solidified state.

Small-strain elasto-plastic deformation

Internally Pressurized Thick-Walled Cylinder





Elastic regime – Navier Cauchy problem

 $(\lambda + \mu) \nabla (\nabla \cdot \vec{u}) + \mu \nabla^2 \vec{u} = 0$

Upon surpassing a critical stress threshold the material experiences localized irreversible plastic deformation – von Mises criterion

 $\begin{cases} \Phi \leq 0, & \text{(elastic deformation), solution is locally valid} \\ \Phi > 0, & \text{(plastic deformation), solution is locally invalid} \\ \Phi = \sigma_{\text{VMS}n} - \sigma_y(\overline{\varepsilon}_n^p) \end{cases}$

plastic regime a correction

$$\vec{u}_{i} = \vec{u}_{i-1} + \delta \vec{u}$$

$$\delta \varepsilon = \frac{\nabla (\delta \vec{u}) + (\nabla (\delta \vec{u}))^{\mathsf{T}}}{2}$$

$$\varepsilon_{i}^{e} = \varepsilon_{i-1}^{e} + \delta \varepsilon$$

$$\varepsilon_{i}^{p} = \varepsilon_{i-1}^{p}$$

$$\overline{\varepsilon}_{i}^{p} = \overline{\varepsilon}_{i-1}^{p}$$

$$\sigma_{i} = \mathbf{D}^{e} \varepsilon_{i}^{e}$$

Return mapping algorithm

$$\Phi = \sigma_{\mathrm{VMS}\,i} - 3\mu\Delta\gamma - \sigma_y(\overline{\varepsilon}_i^p + \Delta\gamma) = 0$$



Displacement magnitude vs radial coordinate – comparison of pure RBF-FD solution with ABAQUS solution

Inertial effects on fluid flow in complex porous media

nertial effects on fluid flow in complex porous media

Body force driven Flow through periodic lattice



D. W. Holmes, J. R. Williams, P. Tilke, Smooth particle hydrodynamics simulations of low reynolds number flows through porous media, International Journal for Numerical and Analytical Methods in Geomechanics 35 (4) (2011) 419–437

Flow through disordered porous media Randomly placed square obstructions on a 64x64 grid



J.S. Andrade, U.M.S. Costa, M.P. Almeida, H.A. Makse, H.E. Stanley, Inertia effectson fluid flow through disordered porous media, The American Physical Society, Physical Review Letters 82 (26) (1999) 5249–5252.



Simulation of overhead power line cooling

Simulation of overhead power line cooling







y[m]

RBF-FD – numerical simulation, M - measurement



End users

Power plant

natural convectio

heat transfer and

generation

Transmission network

Distribution network

Natural convection problem: $\rho^{a} \frac{\partial \mathbf{v}}{\partial t} + \rho^{a} \nabla \cdot (\mathbf{v}\mathbf{v}) = -\nabla P + \nabla \cdot (\mu^{a} \nabla \mathbf{v}) + \mathbf{b}$

$$\nabla \cdot \mathbf{v} = 0$$

$$\rho^{a} c_{p}^{a} \frac{\partial T^{a}}{\partial t} + \rho^{a} c_{p}^{a} \nabla \cdot (T^{a} \mathbf{v}) = \nabla \cdot \left(\lambda^{a} \nabla T^{a}\right)$$

Boundary condition $q_{R} = \sigma_{B}\epsilon_{s} \left(T_{al}^{4}(r_{2}) - T_{a}^{4}\right) \left[\frac{W}{m^{2}}\right]$ $q_{S} = \frac{\alpha_{s}I_{T}}{\pi} \left[\frac{W}{m^{2}}\right],$

$$\begin{aligned} T^{al}\left(r_{1}\right) &= T^{st}\left(r_{1}\right) \\ \lambda^{al}\left.\frac{\partial T^{al}}{\partial \mathbf{n}}\right|_{r} &= \lambda^{st}\left.\frac{\partial T^{st}}{\partial \mathbf{n}}\right|_{r} \end{aligned}$$

Heat transport and generation

$$c_p^{al} \rho^{al} \frac{\partial T^{al}}{\partial t} = \lambda^{al} \nabla^2 T^{al} + \frac{I^2 R \left(T^{al} - S^{al} \right)}{S^{al}}$$

The project is funded by:

• ELES: transmitting energy, maintaining balance.



The transfer capabilities of overhead power lines are limited by the critical power line temperature that depends on the magnitude of the transferred current and the ambient conditions.



Result of Schlieren photography Simulated temperature

Experimental setup

Dynamic thermal rating operational module



Supply minimal current

Comparison of simulated and measured line temperature at Podlog power line in August 2019.

0.2 0.4 0.6 0.8 1.4

1.6 1.8

1.2

Time (h)

10 0





Mesh-free open source project Medusa



selection Engine

Main features:

- Modular design
- Coordinate free and dimension independent implementation
- Support different strong form meshless methods
- Explicit transformation of equations into code
- Minimal overheads due to the programming abstraction
- Tested code

Medusa is C++ template library using

- Eigen library for linear algebra
- Google test testing framework
- XML and HDF5 support for IO
- Nanoflann for spatial-search structures



http://e6.ijs.si/medusa/docs/html

https://gitlab.com/e62Lab/medusa

Conclusions

Meshless methods have some nice properties

- Simplified spatial discretisation
- Suitable for adaptive analysis

Medusa

- tested modular open source library for mesh-free simulations
- dimension independent
- explicit transformation of equations into code
- Supports hp adaptivity



open source meshless project Medusa: Coordinate Free Mehless Method implementation https://gitlab.com/e62Lab/medusa http://e6.ijs.si/medusa/

Future work

- Better marking strategy based on local data regularity
- Better understanding of the effect of the stencil size and shape on the accuracy and stability

• ...

We are open for collaboration

- joint projects
- Student exchange
- Or just working together on fun problems

Thank you for your attention